

Finite Element Approximation for the Dynamics of Fluidic Two-Phase Biomembranes

John W. Barrett[†] Harald Garcke[‡] Robert Nürnberg[†]

Abstract

Biomembranes and vesicles consisting of multiple phases can attain a multitude of shapes, undergoing complex shape transitions. We study a Cahn–Hilliard model on an evolving hypersurface coupled to Navier–Stokes equations on the surface and in the surrounding medium to model these phenomena. The evolution is driven by a curvature energy, modelling the elasticity of the membrane, and by a Cahn–Hilliard type energy, modelling line energy effects. A stable semidiscrete finite element approximation is introduced and, with the help of a fully discrete method, several phenomena occurring for two-phase membranes are computed.

Key words. fluidic membranes, incompressible two-phase Navier–Stokes flow, parametric finite elements, Helfrich energy, spontaneous curvature, local surface area conservation, line energy, surface phase field model, surface Cahn–Hilliard equation, Marangoni-type effects

1 Introduction

In lipid bilayer membranes a large variety of different shapes and complex shape transition behaviour can be observed. Biological membranes are composed of several components, and lateral separation into different phases or domains have been studied in experiments. Mathematical models for biological membranes treat them as a deformable inextensible fluidic surface governed by bending energies, which involve the curvature of the membrane. If different phases occur, these bending energies will depend on the individual phases, and the local shape of the membrane will depend on the phase present locally. It has also been observed that the interfacial energy of the phase boundaries on the membrane can have a pronounced effect on the membrane shape, and might lead to effects like budding and fission. We refer to Baumgart et al. (2003) for experimental studies and to Döbereiner

[†]Department of Mathematics, Imperial College London, London, SW7 2AZ, UK

[‡]Fakultät für Mathematik, Universität Regensburg, 93040 Regensburg, Germany

et al. (1993); Lipowsky (1992); Jülicher and Lipowsky (1996); Veatch and Keller (2003); Baumgart et al. (2005) for further information on membranes with different fluid phases.

There has been a huge interest in the modelling of (two-phase) biomembranes. Both equilibrium shapes, as well as the evolution of membranes, have been studied intensively. However, a model taking the fluidic behaviour of the membrane, the curvature elasticity, the interfacial line energy and the phase separation in a time dependent model into account is missing so far. It is the goal of this paper to present such a model and –which will be the main contribution of this paper– to come up with a stable numerical approximation scheme for the resulting equations. The model will be based on an elastic bending energy of Canham–Evans–Helfrich type and a Ginzburg–Landau energy modelling the interfacial energy. Through their first variation these energy contributions lead to driving forces for the evolution, which is given by a surface Navier–Stokes system, coupled to bulk dissipation of an ambient fluid, and a convective Cahn–Hilliard type equation, which is formulated on the evolving membrane. The fluid part of the model goes back to Arroyo and DeSimone (2009), whereas an evolution based on a Canham–Evans–Helfrich energy coupled to a Ginzburg–Landau energy on the surface has been studied in the context of gradient flows by Elliott and Stinner (2010a,b, 2013); Helmers (2013); Mercker et al. (2013); Helmers (2015); Mercker and Marciniak-Czochra (2015). However, a coupling, which will give the natural dynamics on the interface, is stated here for the first time, and we will show that physically reasonable energy dissipation inequalities hold. Here the dissipation has contributions stemming from viscous friction in the bulk and on the surface, and from dissipation due to diffusion on the membrane.

For the elastic energy we consider the classical Canham–Evans–Helfrich energy

$$\int_{\Gamma} \frac{1}{2} \alpha (\kappa - \overline{\kappa})^2 + \alpha^G \mathcal{K} \, d\mathcal{H}^{d-1}, \quad (1.1)$$

where $\Gamma \subset \mathbb{R}^d$, $d = 2, 3$, is a hypersurface without boundary, $\alpha > 0$ and α^G are the bending and Gaussian bending rigidities, κ is the mean curvature, $\overline{\kappa}$ is the spontaneous curvature, which can be caused by local inhomogeneities within the membrane, \mathcal{K} is the Gaussian curvature and \mathcal{H}^{d-1} is the $(d - 1)$ -dimensional surface Hausdorff measure. As discussed in Nitsche (1993), the most general form of a curvature energy density that is at most quadratic in the principal curvatures and is also symmetric in the principal curvatures has the form $\frac{1}{2} \alpha \kappa^2 + \alpha^G \mathcal{K} + \alpha_1 \kappa + \alpha_2$, which leads to (1.1) by choosing $\alpha_1 = -\alpha \overline{\kappa}$ and $\alpha_2 = \frac{1}{2} \alpha \overline{\kappa}^2$. In the case $d = 2$ the most general form which is at most quadratic in the curvature is $\frac{1}{2} \alpha \kappa^2 + \alpha_1 \kappa + \alpha_2$. Hence throughout this paper we set $\alpha^G = 0$ in the case $d = 2$.

We also introduce an order parameter \mathbf{c} , which takes the values ± 1 in the two different phases, and this parameter is related to the composition of the chemical species within the membrane. On the surface we then use a phase field model to approximate the interfacial energy by the Ginzburg–Landau functional

$$\beta \int_{\Gamma} \frac{1}{2} \gamma |\nabla_s \mathbf{c}|^2 + \gamma^{-1} \Psi(\mathbf{c}) \, d\mathcal{H}^{d-1},$$

where $\beta > 0$ is related to the line tension coefficient and γ is a multiple of the interfacial thickness of the diffusional layer separating the two phases. Furthermore, ∇_s is the surface gradient and Ψ is a double well potential.

In the different phases α , $\bar{\alpha}$ and α^G will take different values, and we will interpolate these values obtaining functions $\alpha(\mathbf{c}) > 0$, $\bar{\alpha}(\mathbf{c})$ and $\alpha^G(\mathbf{c})$. The total energy will hence have the form

$$E(\Gamma, \mathbf{c}) = \int_{\Gamma} b(\boldsymbol{\kappa}, \mathbf{c}) + \alpha^G(\mathbf{c}) \mathcal{K} + \beta b_{CH}(\mathbf{c}) \, d\mathcal{H}^{d-1}, \quad (1.2a)$$

where

$$b(\boldsymbol{\kappa}, \mathbf{c}) = \frac{1}{2} \alpha(\mathbf{c}) (\boldsymbol{\kappa} - \bar{\boldsymbol{\kappa}}(\mathbf{c}))^2 \quad \text{and} \quad b_{CH}(\mathbf{c}) = \frac{1}{2} \gamma |\nabla_s \mathbf{c}|^2 + \gamma^{-1} \Psi(\mathbf{c}). \quad (1.2b)$$

We recall that we assume $\alpha^G = 0$ in the case $d = 2$. In the case $d = 3$, and if α^G is constant, then the contribution $\int_{\Gamma} \alpha^G(\mathbf{c}) \mathcal{K} \, d\mathcal{H}^2$ is constant for a fixed topological type, which is a consequence of the Gauss–Bonnet theorem for closed surfaces,

$$\int_{\Gamma} \mathcal{K} \, d\mathcal{H}^2 = 2\pi m(\Gamma), \quad (1.3)$$

where $m(\Gamma) \in \mathbb{Z}$ denotes the Euler characteristic of Γ . However, if α^G is inhomogeneous, this term plays a role, which was discussed for example in Jülicher and Lipowsky (1996) in the context of two-phase membranes. Here we also mention that the contributions $\frac{1}{2} \int_{\Gamma} \alpha(\mathbf{c}) \boldsymbol{\kappa}^2 \, d\mathcal{H}^2 + \int_{\Gamma} \alpha^G(\mathbf{c}) \mathcal{K} \, d\mathcal{H}^2$ to the energy $E(\Gamma, \mathbf{c})$ are positive semidefinite with respect to the principal curvatures if $\alpha^G(s) \in [-2\alpha(s), 0]$ for all $s \in \mathbb{R}$. On account of the Gauss–Bonnet theorem, (1.3), we hence obtain that the energy $E(\Gamma, \mathbf{c})$ can be bounded from below if $\alpha^G(s) \geq \alpha_{\max}^G - 2\alpha(s)$ for all $s \in \mathbb{R}$, which will hold whenever

$$\alpha_{\min} \geq \frac{1}{2} (\alpha_{\max}^G - \alpha_{\min}^G), \quad (1.4)$$

where $\alpha_{\min} = \min_{s \in \mathbb{R}} \alpha(s)$, and similarly for $\alpha_{\min}^G, \alpha_{\max}^G$. We note that this constraint is likely to have implications for the existence and regularity theory of gradient and related flows for $E(\Gamma, \mathbf{c})$ in the case $d = 3$.

The energy (1.2a) represents a phase field approximation of a two-phase membrane curvature energy with line tension. In the limit $\gamma \rightarrow 0$ the diffusive interface disappears and a sharp interface limit is obtained. Sharp interface limits of phase field approaches to two-phase membranes have been studied with the help of formal asymptotics by Elliott and Stinner (2010b) in the case of a C^1 -limiting surface, and rigorously by Helmers (2013) for axisymmetric two-phase membranes allowing for tangent discontinuities at interfaces. Later Helmers (2015) also showed a rigorous convergence result for the axisymmetric situation in the C^1 -case.

We will now consider a closed membrane, which evolves in time in a domain Ω , separating the domain into regions $\Omega_+(t)$ and $\Omega_-(t) := \Omega \setminus \bar{\Omega}_+(t)$. We hence consider an evolving hypersurface $(\Gamma(t))_{t \in [0, T]}$, where $T > 0$ is a fixed time. We will assume that

the classical Navier–Stokes equations hold in $\Omega_-(t)$ and $\Omega_+(t)$ and on the membrane we require the conditions

$$[\vec{u}]_-^+ = \vec{0} \quad \text{on } \Gamma(t), \quad (1.5a)$$

$$\rho_\Gamma \partial_t^\bullet \vec{u} - \nabla_s \cdot \underline{\underline{\sigma}}_\Gamma = [\underline{\underline{\sigma}} \vec{\nu}]_-^+ + \vec{f}_\Gamma \quad \text{on } \Gamma(t), \quad (1.5b)$$

$$\nabla_s \cdot \vec{u} = 0 \quad \text{on } \Gamma(t), \quad (1.5c)$$

$$\vec{\mathcal{V}} \cdot \vec{\nu} = \vec{u} \cdot \vec{\nu} \quad \text{on } \Gamma(t), \quad (1.5d)$$

where \vec{u} is the fluid velocity, $\vec{\mathcal{V}}$ is the interface velocity, $\vec{\nu}$ is a unit normal to $\Gamma(t)$, $\rho_\Gamma \in \mathbb{R}_{\geq 0}$ denotes the surface material density and the source term $\vec{f}_\Gamma = -\delta E / \delta \Gamma$ is the first variation of the total energy of $\Gamma(t)$ with respect to Γ , and will be stated in (2.4) below in detail. In addition, $\nabla_s \cdot$ denotes the surface divergence on $\Gamma(t)$, and the surface stress tensor is given by

$$\underline{\underline{\sigma}}_\Gamma = 2\mu_\Gamma \underline{\underline{D}}_s(\vec{u}) - p_\Gamma \underline{\underline{\mathcal{P}}}_\Gamma \quad \text{on } \Gamma(t), \quad (1.6)$$

where $\mu_\Gamma \in \mathbb{R}_{\geq 0}$ is the interfacial shear viscosity and p_Γ denotes the surface pressure, which acts as a Lagrange multiplier for the incompressibility condition (1.5c). Here

$$\underline{\underline{\mathcal{P}}}_\Gamma = \underline{\underline{\text{Id}}} - \vec{\nu} \otimes \vec{\nu} \quad \text{on } \Gamma(t), \quad (1.7a)$$

with $\underline{\underline{\text{Id}}} \in \mathbb{R}^{d \times d}$ denoting the identity matrix, and

$$\underline{\underline{D}}_s(\vec{u}) = \frac{1}{2} \underline{\underline{\mathcal{P}}}_\Gamma (\nabla_s \vec{u} + (\nabla_s \vec{u})^T) \underline{\underline{\mathcal{P}}}_\Gamma \quad \text{on } \Gamma(t), \quad (1.7b)$$

where the surface gradient $\nabla_s = \underline{\underline{\mathcal{P}}}_\Gamma \nabla = (\partial_{s_1}, \dots, \partial_{s_d})$ on $\Gamma(t)$, and $\nabla_s \vec{u} = (\partial_{s_j} u_i)_{i,j=1}^d$. Similarly, the bulk stress tensor in (1.5b) is defined by

$$\underline{\underline{\sigma}} = \mu (\nabla \vec{u} + (\nabla \vec{u})^T) - p \underline{\underline{\text{Id}}} = 2\mu \underline{\underline{D}}(\vec{u}) - p \underline{\underline{\text{Id}}}, \quad (1.8)$$

where $\underline{\underline{D}}(\vec{u}) := \frac{1}{2} (\nabla \vec{u} + (\nabla \vec{u})^T)$ is the bulk rate-of-deformation tensor, with $\nabla \vec{u} = (\partial_{x_j} u_i)_{i,j=1}^d$. Moreover, p is the bulk pressure and $\mu(t) = \mu_+ \mathcal{X}_{\Omega_+(t)} + \mu_- \mathcal{X}_{\Omega_-(t)}$, with $\mu_\pm \in \mathbb{R}_{>0}$, denotes the dynamic viscosities in the two phases, where here and throughout $\mathcal{X}_\mathcal{A}$ defines the characteristic function for a set \mathcal{A} . Moreover, as usual, $[\vec{u}]_-^+ := \vec{u}_+ - \vec{u}_-$ and $[\underline{\underline{\sigma}} \vec{\nu}]_-^+ := \underline{\underline{\sigma}}_+ \vec{\nu} - \underline{\underline{\sigma}}_- \vec{\nu}$ denote the jumps in velocity and normal stress across the interface $\Gamma(t)$. Here and throughout, we employ the shorthand notation $\vec{a}_\pm := \vec{a}|_{\Omega_\pm(t)}$ for a function $\vec{a} : \Omega \times [0, T] \rightarrow \mathbb{R}^d$; and similarly for scalar and matrix-valued functions. In addition,

$$\partial_t^\bullet \zeta = \zeta_t + \vec{u} \cdot \nabla \zeta \quad (1.9)$$

denotes the material time derivative of ζ on $\Gamma(t)$, see e.g. Dziuk and Elliott (2013, p. 324).

The overall model is completed by the following Cahn–Hilliard dynamics on $\Gamma(t)$

$$\vartheta \partial_t^\bullet \mathbf{c} = \Delta_s \mathbf{m}, \quad (1.10a)$$

$$\mathbf{m} = -\beta \gamma \Delta_s \mathbf{c} + \beta \gamma^{-1} \Psi'(\mathbf{c}) + b_{,\mathbf{c}}(\boldsymbol{\varkappa}, \mathbf{c}) + (\alpha^G)'(\mathbf{c}) \mathcal{K}, \quad (1.10b)$$

where \mathbf{m} denotes the chemical potential, $\Delta_s = \nabla_s \cdot \nabla_s$ is the Laplace–Beltrami operator and $\vartheta \in \mathbb{R}_{>0}$ is a kinetic coefficient. We note here that $\mathbf{m} = \delta E / \delta \mathbf{c}$ is the first variation of the total energy with respect to \mathbf{c} , see Sections 2, 3 and the Appendix for more details. Equation (1.10a) is a convection-diffusion equation for the species concentration on an evolving surface driven by the chemical potential \mathbf{m} . For more information on the Cahn–Hilliard equation we refer to Elliott (1989); Novick-Cohen (2008). We note that the Cahn–Hilliard equation on an evolving surface was studied by Elliott and Ranner (2015), including its finite element approximation.

It turns out that the overall model with suitable boundary conditions, e.g. $\vec{u} = 0$ on $\partial\Omega$, fulfils, in the case where the outer forces are zero, the following dissipation identity

$$\begin{aligned} \frac{d}{dt} \left(\frac{1}{2} \int_{\Omega} \rho |\vec{u}|^2 d\mathcal{L}^d + \frac{1}{2} \int_{\Gamma(t)} \rho_{\Gamma} |\vec{u}|^2 d\mathcal{H}^{d-1} + E(\Gamma(t), \mathbf{c}(t)) \right) \\ + 2 \int_{\Omega} \mu |\underline{D}(\vec{u})|^2 d\mathcal{L}^d + 2 \mu_{\Gamma} \int_{\Gamma(t)} |\underline{D}_s(\vec{u})|^2 d\mathcal{H}^{d-1} + \theta^{-1} \int_{\Gamma(t)} |\nabla_s \mathbf{m}|^2 d\mathcal{H}^{d-1} = 0, \end{aligned} \quad (1.11)$$

which is consistent with the second law of thermodynamics in its isothermal formulation. The fourth and fifth term in (1.11) describe dissipation by viscous friction in the bulk and on the surface, and the last term models dissipation due to diffusion of molecules on the surface. We also note that the introduced model conserves the volume of the bulk phases, the surface area and the total species concentration on the surface, i.e.

$$\frac{d}{dt} |\Omega^-(t)| = \frac{d}{dt} \mathcal{H}^{d-1}(\Gamma(t)) = \frac{d}{dt} \int_{\Gamma(t)} \mathbf{c}(t) d\mathcal{H}^{d-1} = 0. \quad (1.12)$$

In particular, in contrast to other works, no artificial Lagrange multipliers are needed to conserve the enclosed volume, the total surface area and the total species concentration.

It is one of the main goals of this contribution to introduce and analyze a numerical method that fulfils discrete variants of the dissipation inequality and of the conservation properties (1.12), see the results in Theorem 4.2 and Theorem 4.3, below.

Let us now discuss related works on two-phase membranes. The interest in two-phase membranes increased due to the fascinating work of Baumgart et al. (2003, 2005), as experiments seem to validate earlier theories by Lipowsky (1992); Jülicher and Lipowsky (1996) on two-phase membranes, and showed an amazing multitude of complex shapes and patterns. There have been many studies on two-phase axisymmetric two-phase membranes, both from an analytical and from a numerical point of view, see Jülicher and Lipowsky (1996); Helmers (2011, 2013, 2015); Choksi et al. (2013); Cox and Lowengrub (2015), and the references therein. However, only very few works study general shapes of two-phase membranes from a theoretical or computational point of view. In this context we refer to Wang and Du (2008); Lowengrub et al. (2009); Das et al. (2009); Elliott and Stinner (2010a,b); Mercker et al. (2012); Elliott and Stinner (2013); Tu (2013); Mercker et al. (2013); Mercker and Marciniak-Czochra (2015). But we note that none of the above mentioned contributions considered a stability analysis for their numerical approximations. We combine aspects of some of these approaches with the dynamics studied by

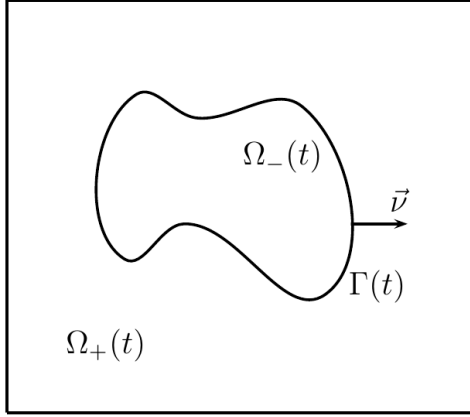


Figure 1: The domain Ω in the case $d = 2$.

Arroyo and DeSimone (2009), and we generalize computational approaches of the present authors for one-phase membranes, see e.g. Barrett et al. (2016a,b), to numerically compute evolving two-phase membranes.

The outline of the paper is as follows. In the following section we introduce the model with all its details. In Section 3 we introduce a weak formulation, which is then discretized in space in Section 4. We then also show that this scheme decreases the total energy and obeys the relevant global conservation properties. In Section 5 we introduce a fully discrete scheme and show existence and uniqueness of a fully discrete solution assuming an LBB condition. In Section 6 we comment on the methods used to solve the fully discrete systems. In Section 7 we present several numerical computations in two and three spatial dimensions, illustrating the properties of the numerical approach and showing the complex interplay between the curvature functional, the Ginzburg–Landau energy and the Navier–Stokes dynamics. In the Appendix we finally state the details of the derivation of the model, and we show that the weak formulation we introduce is consistent with the strong formulation for smooth solutions.

2 Notation and governing equations

In this section we formulate the model, which was sketched in the Introduction, with all its details. Let $\Omega \subset \mathbb{R}^d$ be a given domain, where $d = 2$ or $d = 3$. We seek a time dependent interface $(\Gamma(t))_{t \in [0, T]}$, $\Gamma(t) \subset \Omega$, which for all $t \in [0, T]$ separates Ω into a domain $\Omega_+(t)$, occupied by the outer phase, and a domain $\Omega_-(t) := \Omega \setminus \overline{\Omega_+(t)}$, which is occupied by the inner phase, see Figure 1 for an illustration. For later use, we assume that $(\Gamma(t))_{t \in [0, T]}$ is an evolving hypersurface without boundary that is parameterized by $\vec{x}(\cdot, t) : \Upsilon \rightarrow \mathbb{R}^d$, where $\Upsilon \subset \mathbb{R}^d$ is a given reference manifold, i.e. $\Gamma(t) = \vec{x}(\Upsilon, t)$. Then

$$\vec{\mathcal{V}}(\vec{z}, t) := \vec{x}_t(\vec{q}, t) \quad \forall \vec{z} = \vec{x}(\vec{q}, t) \in \Gamma(t) \quad (2.1)$$

defines the velocity of $\Gamma(t)$, and $\mathcal{V} := \vec{\mathcal{V}} \cdot \vec{\nu}$ is the normal velocity of the evolving hypersurface $\Gamma(t)$, where $\vec{\nu}(t)$ is the unit normal on $\Gamma(t)$ pointing into $\Omega_+(t)$. Moreover, we define the space-time surface $\Gamma_T := \bigcup_{t \in [0, T]} \Gamma(t) \times \{t\}$.

Let $\rho(t) = \rho_+ \chi_{\Omega_+(t)} + \rho_- \chi_{\Omega_-(t)}$, with $\rho_{\pm} \in \mathbb{R}_{\geq 0}$, denote the fluid densities. Denoting by $\vec{u} : \Omega \times [0, T] \rightarrow \mathbb{R}^d$ the fluid velocity, by $p : \Omega \times [0, T] \rightarrow \mathbb{R}$ the pressure, by $\underline{\underline{\sigma}} : \Omega \times [0, T] \rightarrow \mathbb{R}^{d \times d}$ the stress tensor, and by $\vec{f} : \Omega \times [0, T] \rightarrow \mathbb{R}^d$ a possible volume force, the incompressible Navier–Stokes equations in the two phases are given by (1.8) and

$$\rho (\vec{u}_t + (\vec{u} \cdot \nabla) \vec{u}) - \nabla \cdot \underline{\underline{\sigma}} = \rho \vec{f} \quad \text{in } \Omega_{\pm}(t), \quad (2.2a)$$

$$\nabla \cdot \vec{u} = 0 \quad \text{in } \Omega_{\pm}(t), \quad (2.2b)$$

$$\vec{u} = \vec{g} \quad \text{on } \partial_1 \Omega, \quad (2.2c)$$

$$\underline{\underline{\sigma}} \vec{n} = \vec{0} \quad \text{on } \partial_2 \Omega, \quad (2.2d)$$

where $\partial \Omega = \partial_1 \Omega \cup \partial_2 \Omega$, with $\partial_1 \Omega \cap \partial_2 \Omega = \emptyset$, denotes the boundary of Ω with outer unit normal \vec{n} . Hence (2.2c) prescribes a possibly inhomogeneous Dirichlet condition for the velocity on $\partial_1 \Omega$, which collapses to the standard no-slip condition when $\vec{g} = \vec{0}$, while (2.2d) prescribes a stress-free condition on $\partial_2 \Omega$. Throughout this paper we assume that $\mathcal{H}^{d-1}(\partial_1 \Omega) > 0$. We will also assume w.l.o.g. that \vec{g} is extended so that $\vec{g} : \Omega \rightarrow \mathbb{R}^d$. On the free surface $\Gamma(t)$ the conditions (1.5a–d) need to hold, recall the Introduction. The system (2.2a–d), (1.8), (1.5a–d), (1.6) is closed with the initial conditions

$$\Gamma(0) = \Gamma_0, \quad \rho \vec{u}(\cdot, 0) = \rho \vec{u}_0 \quad \text{in } \Omega, \quad \rho_{\Gamma} \vec{u}(\cdot, 0) = \rho_{\Gamma} \vec{u}_0 \quad \text{on } \Gamma_0, \quad (2.3)$$

where $\Gamma_0 \subset \Omega$ and $\vec{u}_0 : \Omega \rightarrow \mathbb{R}^d$ are given initial data satisfying $\rho \nabla \cdot \vec{u}_0 = 0$ in Ω , $\rho_{\Gamma} \nabla_s \cdot \vec{u}_0 = 0$ on Γ_0 and $\rho_+ \vec{u}_0 = \rho_+ \vec{g}$ on $\partial_1 \Omega$. Of course, in the case $\rho_- = \rho_+ = \rho_{\Gamma} = 0$ the initial data \vec{u}_0 is not needed. Similarly, in the case $\rho_- = \rho_+ = 0$ and $\rho_{\Gamma} > 0$ the initial data \vec{u}_0 is only needed on Γ_0 . However, for ease of exposition, and in view of the unfitted nature of our numerical method, we will always assume that \vec{u}_0 , if required, is given on all of Ω .

It is not difficult to show that the conditions (2.2b) enforce volume preservation for the phases, while (1.5c) leads to the conservation of the total surface area $\mathcal{H}^{d-1}(\Gamma(t))$, see (3.6) and (3.7) in Section 3 below for the relevant proofs. As an immediate consequence we obtain that a sphere $\Gamma(t)$ remain a sphere, and that a sphere $\Gamma(t)$ with a zero bulk velocity is a stationary solution.

In addition, the source term \vec{f}_{Γ} in (1.5b) is given by minus the first variation of the energy (1.2a) with respect to Γ , i.e.

$$\begin{aligned} \vec{f}_{\Gamma} = & -\frac{\delta}{\delta \Gamma} E(\Gamma, \mathbf{c}) = [-\Delta_s [\alpha(\mathbf{c}) (\boldsymbol{\kappa} - \overline{\boldsymbol{\kappa}}(\mathbf{c}))] - \alpha(\mathbf{c}) (\boldsymbol{\kappa} - \overline{\boldsymbol{\kappa}}(\mathbf{c})) |\nabla_s \vec{\nu}|^2 + b(\boldsymbol{\kappa}, \mathbf{c}) \boldsymbol{\kappa} \\ & - \nabla_s \cdot ([\boldsymbol{\kappa} \underline{\underline{\text{Id}}} + \nabla_s \vec{\nu}] \nabla_s \alpha^G(\mathbf{c}))] \vec{\nu} + (b_{,\mathbf{c}}(\boldsymbol{\kappa}, \mathbf{c}) + (\alpha^G)'(\mathbf{c}) \mathcal{K}) \nabla_s \mathbf{c} \\ & + \beta [b_{CH}(\mathbf{c}) \boldsymbol{\kappa} \vec{\nu} + \nabla_s b_{CH}(\mathbf{c}) - \gamma \nabla_s \cdot ((\nabla_s \mathbf{c}) \otimes (\nabla_s \mathbf{c}))], \end{aligned} \quad (2.4)$$

where we have defined

$$b_{,\mathbf{c}}(\varkappa, \mathbf{c}) = \frac{\partial}{\partial \mathbf{c}} b(\varkappa, \mathbf{c}) = \frac{1}{2} \alpha'(\mathbf{c}) (\varkappa - \overline{\varkappa}(\mathbf{c}))^2 - \alpha(\mathbf{c}) (\varkappa - \overline{\varkappa}(\mathbf{c})) \overline{\varkappa}'(\mathbf{c}). \quad (2.5)$$

Throughout we assume that $\alpha, \alpha^G \in C^1(\mathbb{R})$, with $\alpha(s) > 0$ for all $s \in \mathbb{R}$. We refer to the appendix for a detailed derivation of (2.4). In contrast to situations where the energy density does not depend on a species concentration, we now have tangential contributions to \vec{f}_Γ . In particular, the terms $(b_{,\mathbf{c}}(\varkappa, \mathbf{c}) + (\alpha^G)'(\mathbf{c}) \mathcal{K}) \nabla_s \mathbf{c} + \beta \nabla_s b_{CH}(\mathbf{c}) - \beta \gamma \nabla_s \cdot ((\nabla_s \mathbf{c}) \otimes (\nabla_s \mathbf{c}))$ give rise to a tangential flow and hence can induce a Marangoni-type effect.

The overall model we are going to study in this work is the coupled bulk and surface Navier–Stokes equations (2.2a–d), (1.8), (1.5a–d), (1.6), (2.3) together with the convective Cahn–Hilliard system (1.10a,b) on the evolving interface, suitably supplemented with initial conditions for \mathbf{c} . Here the double well potential Ψ in (1.2b) and (1.10b) may be chosen, for example, as a quartic potential

$$\Psi(s) = \frac{1}{4} (s^2 - 1)^2, \quad (2.6a)$$

or as the obstacle potential

$$\Psi(s) := \begin{cases} \frac{1}{2} (1 - s^2) & \text{if } |s| \leq 1, \\ \infty & \text{if } |s| > 1, \end{cases} \quad (2.6b)$$

which restricts $\mathbf{c} \in [-1, 1]$. For the analysis we will always assume that $\Psi \in C^1(\mathbb{R})$ for ease of exposition, but we will use (2.6b) for our fully discrete approximations.

As stated previously, \varkappa in (2.4) denotes the so-called mean curvature of $\Gamma(t)$, i.e. the sum of the principal curvatures \varkappa_i , $i = 1, \dots, d-1$, of $\Gamma(t)$, where we have adopted the sign convention that \varkappa is negative where $\Omega_-(t)$ is locally convex. In particular, it holds that

$$\Delta_s \vec{\text{id}} = \varkappa \vec{\nu} =: \vec{\varkappa} \quad \text{on } \Gamma(t), \quad (2.7)$$

where $\vec{\text{id}}$ is the identity function on \mathbb{R}^d . For later use, we recall that the second fundamental tensor for $\Gamma(t)$ is given by $\nabla_s \vec{\nu}$. Moreover, we note that $-\nabla_s \vec{\nu}(\vec{z})$, for any $\vec{z} \in \Gamma(t)$, is a symmetric linear map that has a zero eigenvalue with eigenvector $\vec{\nu}$, i.e.

$$(\nabla_s \vec{\nu})^T = \nabla_s \vec{\nu} \quad \text{and} \quad (\nabla_s \vec{\nu}) \vec{\nu} = \vec{0}, \quad (2.8)$$

and the remaining $(d-1)$ eigenvalues, $\varkappa_1, \dots, \varkappa_{d-1}$, are the principal curvatures of Γ at \vec{z} ; see e.g. (Deckelnick et al., 2005, p. 152). The mean curvature \varkappa and the Gauss curvature \mathcal{K} can now be stated as

$$\varkappa = -\text{tr}(\nabla_s \vec{\nu}) = -\nabla_s \cdot \vec{\nu} = \sum_{i=1}^{d-1} \varkappa_i \quad \text{and} \quad \mathcal{K} = \prod_{i=1}^{d-1} \varkappa_i, \quad (2.9)$$

which in the case $d = 3$ immediately yields that

$$\mathcal{K} = \frac{1}{2} (\varkappa^2 - |\nabla_s \vec{\nu}|^2). \quad (2.10)$$

We recall that in the case $d = 2$, we always assume that $\alpha^G = 0$. In the case $d = 3$, on the other hand, we have from (2.10) that

$$\int_{\Gamma(t)} \alpha^G(\mathbf{c}) \mathcal{K} \, d\mathcal{H}^{d-1} = \frac{1}{2} \int_{\Gamma(t)} \alpha^G(\mathbf{c}) (|\vec{\mathcal{Z}}|^2 - |\underline{\underline{w}}|^2) \, d\mathcal{H}^{d-1}, \quad (2.11)$$

where $\underline{\underline{w}} \in [H^1(\Gamma(t))]^{d \times d}$ is such that for all $\underline{\underline{\zeta}} \in [H^1(\Gamma(t))]^{d \times d}$

$$\int_{\Gamma(t)} \underline{\underline{w}} : \underline{\underline{\zeta}} \, d\mathcal{H}^{d-1} = \int_{\Gamma(t)} \nabla_s \vec{\nu} : \underline{\underline{\zeta}} \, d\mathcal{H}^{d-1} = - \int_{\Gamma(t)} \vec{\nu} \cdot (\nabla_s \cdot \underline{\underline{\zeta}}) + \vec{\nu} \cdot (\underline{\underline{\zeta}} \vec{\mathcal{Z}}) \, d\mathcal{H}^{d-1}. \quad (2.12)$$

Here we have recalled from Dziuk and Elliott (2013, Theorem 2.10) that

$$\begin{aligned} \langle \nabla_s \zeta, \vec{\eta} \rangle_{\Gamma(t)} + \langle \zeta, \nabla_s \cdot \vec{\eta} \rangle_{\Gamma(t)} &= \langle \nabla_s \cdot (\zeta \vec{\eta}), 1 \rangle_{\Gamma(t)} = - \langle \zeta \varkappa \vec{\nu}, \vec{\eta} \rangle_{\Gamma(t)} \\ &\quad \forall \zeta \in H^1(\Gamma(t)), \vec{\eta} \in [H^1(\Gamma(t))]^d. \end{aligned} \quad (2.13)$$

Hence the total energy $E(\Gamma(t), \mathbf{c}(t))$, on recalling (1.2a,b), can be rewritten as

$$E(\Gamma(t), \mathbf{c}(t)) = \int_{\Gamma} \frac{1}{2} \alpha(\mathbf{c}) |\vec{\mathcal{Z}} - \vec{\mathcal{Z}}(\mathbf{c}) \vec{\nu}|^2 + \frac{1}{2} \alpha^G(\mathbf{c}) (|\vec{\mathcal{Z}}|^2 - |\underline{\underline{w}}|^2) + \beta b_{CH}(\mathbf{c}) \, d\mathcal{H}^{d-1}, \quad (2.14)$$

where $\underline{\underline{w}}$ is given by (2.12), and where $\vec{\mathcal{Z}}$, on recalling (2.13), can be defined by

$$\langle \vec{\mathcal{Z}}, \vec{\eta} \rangle_{\Gamma(t)} + \left\langle \nabla_s \text{id}, \nabla_s \vec{\eta} \right\rangle_{\Gamma(t)} = 0 \quad \forall \vec{\eta} \in [H^1(\Gamma(t))]^d. \quad (2.15)$$

3 Weak formulation

We begin by recalling the weak formulation of (2.2a–d), (1.8), (1.5a–d), (1.6) from Barrett et al. (2016a). To this end, we introduce the following function spaces for a given $\vec{a} \in [H^1(\Omega)]^d$:

$$\begin{aligned} \mathbb{U}(\vec{a}) &:= \{\vec{\varphi} \in [H^1(\Omega)]^d : \vec{\varphi} = \vec{a} \text{ on } \partial_1 \Omega\}, \quad \mathbb{V}(\vec{a}) := L^2(0, T; \mathbb{U}(\vec{a})) \cap H^1(0, T; [L^2(\Omega)]^d), \\ \mathbb{V}_{\Gamma}(\vec{a}) &:= \{\vec{\varphi} \in \mathbb{V}(\vec{a}) : \vec{\varphi}|_{\Gamma_T} \in [H^1(\Gamma_T)]^d\}. \end{aligned} \quad (3.1a)$$

In addition, we let $\mathbb{P} := L^2(\Omega)$ and define

$$\widehat{\mathbb{P}} := \begin{cases} \{\eta \in \mathbb{P} : \int_{\Omega} \eta \, d\mathcal{L}^d = 0\} & \text{if } \mathcal{H}^{d-1}(\partial_2 \Omega) = 0, \\ \mathbb{P} & \text{if } \mathcal{H}^{d-1}(\partial_2 \Omega) > 0. \end{cases} \quad (3.1b)$$

Here and throughout, \mathcal{H}^{d-1} denotes the $(d-1)$ -dimensional Hausdorff measure in \mathbb{R}^d , while \mathcal{L}^d denotes the Lebesgue measure in \mathbb{R}^d . Moreover, we let (\cdot, \cdot) and $\langle \cdot, \cdot \rangle_{\partial_2 \Omega}$ denote the L^2 -inner products on Ω and $\partial_2 \Omega$, and similarly for $\langle \cdot, \cdot \rangle_{\Gamma(t)}$.

Similarly to (1.9) we define the following time derivative that follows the parameterization $\vec{x}(\cdot, t)$ of $\Gamma(t)$, rather than \vec{u} . In particular, we let

$$\partial_t^\circ \zeta = \zeta_t + \vec{\nu} \cdot \nabla \zeta \quad \forall \zeta \in H^1(\Gamma_T); \quad (3.2)$$

where we stress that this definition is well-defined, even though ζ_t and $\nabla \zeta$ do not make sense separately for a function $\zeta \in H^1(\Gamma_T)$. On recalling (1.9) we obtain that $\partial_t^\circ = \partial_t^\bullet$ if $\vec{\mathcal{V}} = \vec{u}$ on $\Gamma(t)$. Moreover, for later use we note that

$$\frac{d}{dt} \langle \chi, \zeta \rangle_{\Gamma(t)} = \langle \partial_t^\circ \chi, \zeta \rangle_{\Gamma(t)} + \langle \chi, \partial_t^\circ \zeta \rangle_{\Gamma(t)} + \left\langle \chi \zeta, \nabla_s \cdot \vec{\mathcal{V}} \right\rangle_{\Gamma(t)} \quad \forall \chi, \zeta \in H^1(\Gamma_T), \quad (3.3)$$

see Dziuk and Elliott (2013, Lem. 5.2).

The weak formulation of (2.2a–d), (1.8), (1.5a–d), (1.6), with $E(\Gamma(t), \mathbf{c}(t))$ replaced by $\frac{1}{2} \alpha \langle \vec{\mathcal{Z}}, \vec{\mathcal{Z}} \rangle_{\Gamma(t)}$, from Barrett et al. (2016a) is then given as follows. Find $\Gamma(t) = \vec{x}(\Upsilon, t)$ for $t \in [0, T]$ with $\vec{\mathcal{V}} \in [L^2(\Gamma_T)]^d$ and $\vec{\mathcal{V}}(\cdot, t) \in [H^1(\Gamma(t))]^d$ for almost all $t \in (0, T)$, and functions $\vec{u} \in \mathbb{V}_\Gamma(\vec{g})$, $p \in L^2(0, T; \widehat{\mathbb{P}})$, $p_\Gamma \in L^2(\Gamma_T)$, $\vec{\mathcal{Z}} \in [H^1(\Gamma_T)]^d$ and $\vec{f}_\Gamma \in [L^2(\Gamma_T)]^d$ such that the initial conditions (2.3) hold and such that for almost all $t \in (0, T)$ it holds that

$$\begin{aligned} \frac{1}{2} \left[\frac{d}{dt} (\rho \vec{u}, \vec{\xi}) + (\rho \vec{u}_t, \vec{\xi}) - (\rho \vec{u}, \vec{\xi}_t) + (\rho, [(\vec{u} \cdot \nabla) \vec{u}] \cdot \vec{\xi} - [(\vec{u} \cdot \nabla) \vec{\xi}] \cdot \vec{u}) + \rho_+ \left\langle \vec{u} \cdot \vec{n}, \vec{u} \cdot \vec{\xi} \right\rangle_{\partial_2 \Omega} \right] \\ + 2 (\mu \underline{\underline{D}}(\vec{u}), \underline{\underline{D}}(\vec{\xi})) - (p, \nabla \cdot \vec{\xi}) + \rho_\Gamma \left\langle \partial_t^\circ \vec{u}, \vec{\xi} \right\rangle_{\Gamma(t)} + 2 \mu_\Gamma \left\langle \underline{\underline{D}}_s(\vec{u}), \underline{\underline{D}}_s(\vec{\xi}) \right\rangle_{\Gamma(t)} \\ - \left\langle p_\Gamma, \nabla_s \cdot \vec{\xi} \right\rangle_{\Gamma(t)} = (\rho \vec{f}, \vec{\xi}) + \left\langle \vec{f}_\Gamma, \vec{\xi} \right\rangle_{\Gamma(t)} \quad \forall \vec{\xi} \in \mathbb{V}_\Gamma(\vec{0}), \end{aligned} \quad (3.4a)$$

$$(\nabla \cdot \vec{u}, \varphi) = 0 \quad \forall \varphi \in \widehat{\mathbb{P}}, \quad (3.4b)$$

$$\langle \nabla_s \cdot \vec{u}, \eta \rangle_{\Gamma(t)} = 0 \quad \forall \eta \in L^2(\Gamma(t)), \quad (3.4c)$$

$$\left\langle \vec{\mathcal{V}} - \vec{u}, \vec{\chi} \right\rangle_{\Gamma(t)} = 0 \quad \forall \vec{\chi} \in [L^2(\Gamma(t))]^d, \quad (3.4d)$$

as well as

$$\langle \vec{\mathcal{Z}}, \vec{\eta} \rangle_{\Gamma(t)} + \left\langle \nabla_s \vec{\mathcal{Z}}, \nabla_s \vec{\eta} \right\rangle_{\Gamma(t)} = 0 \quad \forall \vec{\eta} \in [H^1(\Gamma(t))]^d, \quad (3.5a)$$

$$\begin{aligned} \left\langle \vec{f}_\Gamma, \vec{\chi} \right\rangle_{\Gamma(t)} = \alpha \langle \nabla_s \vec{\mathcal{Z}}, \nabla_s \vec{\chi} \rangle_{\Gamma(t)} + \alpha \langle \nabla_s \cdot \vec{\mathcal{Z}}, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} + \frac{1}{2} \alpha \langle |\vec{\mathcal{Z}}|^2, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} \\ - 2 \alpha \left\langle (\nabla_s \vec{\mathcal{Z}})^T, \underline{\underline{D}}_s(\vec{\chi}) (\nabla_s \vec{\mathcal{Z}})^T \right\rangle_{\Gamma(t)} \quad \forall \vec{\chi} \in [H^1(\Gamma(t))]^d, \end{aligned} \quad (3.5b)$$

where in (3.4d) we have recalled (2.1).

For the case $\vec{g} = \vec{0}$, it was shown in Barrett et al. (2016a) that choosing $\vec{\xi} = \vec{u} \in \mathbb{V}_\Gamma(\vec{0})$ in (3.4a), $\varphi = p(\cdot, t) \in \widehat{\mathbb{P}}$ in (3.4b), $\eta = p_\Gamma(\cdot, t) \in L^2(\Gamma(t))$, $\vec{\chi} = \vec{f}_\Gamma$ in (3.4d) and $\vec{\chi} = \vec{\mathcal{V}}$ in (3.5b) yields that

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \left(\|\rho^{\frac{1}{2}} \vec{u}\|_0^2 + \rho_\Gamma \langle \vec{u}, \vec{u} \rangle_{\Gamma(t)} + \alpha \langle \vec{\mathcal{Z}}, \vec{\mathcal{Z}} \rangle_{\Gamma(t)} \right) + 2 \|\mu^{\frac{1}{2}} \underline{\underline{D}}(\vec{u})\|_0^2 + 2 \mu_\Gamma \langle \underline{\underline{D}}_s(\vec{u}), \underline{\underline{D}}_s(\vec{u}) \rangle_{\Gamma(t)} \\ + \frac{1}{2} \rho_+ \langle \vec{u} \cdot \vec{n}, |\vec{u}|^2 \rangle_{\partial_2 \Omega} = (\rho \vec{f}, \vec{u}). \end{aligned}$$

Moreover, we recall from Barrett et al. (2016a) that it follows from (3.3) and (3.4c,d) that

$$\frac{d}{dt} \mathcal{H}^{d-1}(\Gamma(t)) = \frac{d}{dt} \langle 1, 1 \rangle_{\Gamma(t)} = \left\langle 1, \nabla_s \cdot \vec{\mathcal{V}} \right\rangle_{\Gamma(t)} = \langle 1, \nabla_s \cdot \vec{u} \rangle_{\Gamma(t)} = 0, \quad (3.6)$$

while Deckelnick et al. (2005, Lemma 2.1), (3.4b,d) and (3.1b) imply that

$$\frac{d}{dt} \mathcal{L}^d(\Omega_-(t)) = \left\langle \vec{\mathcal{V}}, \vec{\nu} \right\rangle_{\Gamma(t)} = \langle \vec{u}, \vec{\nu} \rangle_{\Gamma(t)} = \int_{\Omega_-(t)} \nabla \cdot \vec{u} \, d\mathcal{L}^d = 0. \quad (3.7)$$

3.1 The first variation of $E(\Gamma(t), \mathbf{c}(t))$

In this section we would like to derive a weak formulation for the first variation of $E(\Gamma(t), \mathbf{c}(t))$ with respect to $\Gamma(t) = \vec{x}(\Upsilon, t)$. To this end, for a given $\vec{\chi} \in [H^1(\Gamma(t))]^d$ and for $\varepsilon \in (0, \varepsilon_0)$, where $\varepsilon_0 \in \mathbb{R}_{>0}$, let $\vec{\Phi}(\cdot, \varepsilon)$ be a family of transformations such that

$$\Gamma_\varepsilon(t) := \{\vec{\Phi}(\vec{z}, \varepsilon) : \vec{z} \in \Gamma(t)\}, \quad \text{where} \quad \vec{\Phi}(\vec{z}, 0) = \vec{z} \text{ and } \frac{\partial \vec{\Phi}}{\partial \varepsilon}(\vec{z}, 0) = \vec{\chi}(\vec{z}) \quad \forall \vec{z} \in \Gamma(t). \quad (3.8)$$

Then the first variation of $\mathcal{H}^{d-1}(\Gamma(t))$ with respect to $\Gamma(t)$ in the direction $\vec{\chi} \in [H^1(\Gamma(t))]^d$ is given by

$$\begin{aligned} \left[\frac{\delta}{\delta \Gamma} \mathcal{H}^{d-1}(\Gamma(t)) \right] (\vec{\chi}) &= \frac{d}{d\varepsilon} \mathcal{H}^{d-1}(\Gamma_\varepsilon(t)) \big|_{\varepsilon=0} = \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} [\mathcal{H}^{d-1}(\Gamma_\varepsilon(t)) - \mathcal{H}^{d-1}(\Gamma(t))] \\ &= \left\langle \nabla_s \text{id}, \nabla_s \vec{\chi} \right\rangle_{\Gamma(t)} = \langle 1, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)}, \end{aligned} \quad (3.9)$$

see e.g. the proof of Lemma 1 in Dziuk (2008). For any quantity w , that is naturally defined on $\Gamma_\varepsilon(t)$, we define

$$\partial_\varepsilon^0 w(\vec{z}) = \frac{d}{d\varepsilon} w_\varepsilon(\vec{\Phi}(\vec{z}, \varepsilon)) \big|_{\varepsilon=0} \quad \forall \vec{z} \in \Gamma(t), \quad (3.10)$$

and similarly for $\partial_\varepsilon^0 \vec{w}$ and $\partial_\varepsilon^0 \underline{w}$. A common example is $\vec{\nu}_\varepsilon$, the outer normal on $\Gamma_\varepsilon(t)$. In cases where $w \in L^\infty(\Gamma(t))$ is meaningful only on $\Gamma(t)$, we let $w_\varepsilon \in L^\infty(\Gamma_\varepsilon(t))$ be such that

$$w_\varepsilon(\vec{\Phi}(\vec{z}, \varepsilon)) = w(\vec{z}) \quad \forall \vec{z} \in \Gamma(t), \quad (3.11)$$

which immediately implies that for such w it holds that $\partial_\varepsilon^0 w = 0$. Once again, we extend (3.11) also to vector- and tensor-valued functions. For later use we note that generalized variants of (3.9) also hold. Similarly to (3.3) it holds that

$$\left[\frac{\delta}{\delta \Gamma} \langle w, v \rangle_{\Gamma(t)} \right] (\vec{\chi}) = \langle \partial_\varepsilon^0 w, v \rangle_{\Gamma(t)} + \langle w, \partial_\varepsilon^0 v \rangle_{\Gamma(t)} + \langle w v, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} \quad \forall w, v \in L^\infty(\Gamma(t)). \quad (3.12)$$

Similarly, it holds that

$$\begin{aligned} \left[\frac{\delta}{\delta \Gamma} \langle \vec{w}, \vec{\nu} \rangle_{\Gamma(t)} \right] (\vec{\chi}) &= \frac{d}{d\varepsilon} \langle \vec{w}_\varepsilon, \vec{\nu}_\varepsilon \rangle_{\Gamma_\varepsilon(t)} \big|_{\varepsilon=0} = \langle \partial_\varepsilon^0 \vec{w}, \vec{\nu} \rangle_{\Gamma(t)} + \langle \vec{w}, \partial_\varepsilon^0 \vec{\nu} \rangle_{\Gamma(t)} \\ &\quad + \langle \vec{w} \cdot \vec{\nu}, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} \quad \forall \vec{w} \in [L^\infty(\Gamma(t))]^d, \end{aligned} \quad (3.13)$$

where $\vec{\nu}_\varepsilon(t)$ denotes the unit normal on $\Gamma_\varepsilon(t)$. In this regard, we note the following result concerning the variation of $\vec{\nu}$, with respect to $\Gamma(t)$, in the direction $\vec{\chi} \in [H^1(\Gamma(t))]^d$:

$$\partial_\varepsilon^0 \vec{\nu} = -[\nabla_s \vec{\chi}]^T \vec{\nu} \quad \text{on} \quad \Gamma(t) \quad \Rightarrow \quad \partial_t^\circ \vec{\nu} = -[\nabla_s \vec{\mathcal{V}}]^T \vec{\nu} \quad \text{on} \quad \Gamma(t), \quad (3.14)$$

see Schmidt and Schulz (2010, Lemma 9). Next we note that for $\vec{\eta} \in [H^1(\Gamma(t))]^d$ it holds that

$$\begin{aligned} \left[\frac{\delta}{\delta \Gamma} \left\langle \nabla_s \text{id}, \nabla_s \vec{\eta} \right\rangle_{\Gamma(t)} \right] (\vec{\chi}) &= \frac{d}{d\varepsilon} \left\langle \nabla_s \text{id}, \nabla_s \vec{\eta}_\varepsilon \right\rangle_{\Gamma_\varepsilon(t)} \Big|_{\varepsilon=0} = \left\langle \nabla_s \cdot \vec{\eta}, \nabla_s \cdot \vec{\chi} \right\rangle_{\Gamma(t)} \\ &+ \sum_{l,m=1}^d \left[\left\langle (\vec{\nu})_l (\vec{\nu})_m \nabla_s (\vec{\eta})_m, \nabla_s (\vec{\chi})_l \right\rangle_{\Gamma(t)} - \left\langle (\nabla_s)_m (\vec{\eta})_l, (\nabla_s)_l (\vec{\chi})_m \right\rangle_{\Gamma(t)} \right] \\ &= \left\langle \nabla_s \vec{\eta}, \nabla_s \vec{\chi} \right\rangle_{\Gamma(t)} + \left\langle \nabla_s \cdot \vec{\eta}, \nabla_s \cdot \vec{\chi} \right\rangle_{\Gamma(t)} - 2 \left\langle (\nabla_s \vec{\eta})^T, \underline{\underline{D}}_s(\vec{\chi}) (\nabla_s \text{id})^T \right\rangle_{\Gamma(t)}, \end{aligned} \quad (3.15)$$

where $\partial_\varepsilon^0 \vec{\eta} = \vec{0}$. We refer to Lemma 2 and the proof of Lemma 3 in Dziuk (2008) for a proof of (3.15). Here we observe that our notation is such that $\nabla_s \vec{\chi} = (\nabla_\Gamma \vec{\chi})^T$, with $\nabla_\Gamma \vec{\chi} = (\partial_{s_i} \chi_j)_{i,j=1}^d$ defined as in Dziuk (2008). Moreover, it holds, on noting (1.7a), that

$$\nabla_s \vec{\chi} \underline{\underline{P}}_\Gamma = \nabla_s \vec{\chi} \quad \Rightarrow \quad \underline{\underline{P}}_\Gamma (\nabla_s \vec{\chi})^T = (\nabla_s \vec{\chi})^T \quad (3.16a)$$

and

$$2 (\nabla_s \vec{\eta})^T : \underline{\underline{D}}_s(\vec{\chi}) (\nabla_s \vec{\phi})^T = (\nabla_s \vec{\eta})^T : [\nabla_s \vec{\chi} + (\nabla_s \vec{\chi})^T] (\nabla_s \vec{\phi})^T, \quad (3.16b)$$

which yields that the last term on the right hand side in (3.15) can be rewritten as in Dziuk (2008).

As $\nabla_s \text{id} = \underline{\underline{P}}_\Gamma$, one can deduce from (1.7a), (3.15) and (3.12) that for sufficiently smooth $\vec{\eta}$

$$\begin{aligned} \partial_\varepsilon^0 (\nabla_s \cdot \vec{\eta}) &= \partial_\varepsilon^0 (\nabla_s \text{id} : \nabla_s \vec{\eta}) = \nabla_s \vec{\eta} : \nabla_s \vec{\chi} - 2 (\nabla_s \vec{\eta})^T : \underline{\underline{D}}_s(\vec{\chi}) (\nabla_s \text{id})^T \\ &= [\nabla_s \vec{\chi} - 2 \underline{\underline{D}}_s(\vec{\chi})] : \nabla_s \vec{\eta} \quad \text{a.e. on} \quad \Gamma(t), \end{aligned} \quad (3.17)$$

where $\partial_\varepsilon^0 \vec{\eta} = \vec{0}$. From (3.17) we can also derive that for sufficiently smooth w

$$\partial_\varepsilon^0 (\nabla_s w) = [\nabla_s \vec{\chi} - 2 \underline{\underline{D}}_s(\vec{\chi})] \nabla_s w \quad \text{a.e. on} \quad \Gamma(t), \quad (3.18)$$

where $\partial_\varepsilon^0 w = 0$. In addition, it follows from (3.18) that

$$\begin{aligned} \partial_\varepsilon^0 |\nabla_s w|^2 &= 2 \nabla_s w \cdot \partial_\varepsilon^0 (\nabla_s w) = -2 \nabla_s w \cdot (\nabla_s \vec{\chi} \nabla_s w) \\ &= -2 (\nabla_s w \otimes \nabla_s w) : \nabla_s \vec{\chi} \quad \text{a.e. on} \quad \Gamma(t), \end{aligned} \quad (3.19)$$

where $\partial_\varepsilon^0 w = 0$.

REMARK. 3.1. We note from (3.17) that the last term in (3.15) can be simplified to

$$-2 \left\langle \nabla_s \vec{\eta}, \underline{\underline{D}}_s(\vec{\chi}) \right\rangle_{\Gamma(t)}. \quad (3.20)$$

However, to be consistent with our approximations in Barrett et al. (2016c), we prefer the form used in (3.15).

It is straightforward to derive results for the time derivative of the considered quantities from the collected first variations above. For example, it follows from (3.15) that

$$\begin{aligned} \frac{d}{dt} \left\langle \nabla_s \vec{\text{id}}, \nabla_s \vec{\eta} \right\rangle_{\Gamma(t)} &= \left\langle \nabla_s \cdot \vec{\eta}, \nabla_s \cdot \vec{\mathcal{V}} \right\rangle_{\Gamma(t)} + \left\langle \nabla_s \vec{\eta}, \nabla_s \vec{\mathcal{V}} \right\rangle_{\Gamma(t)} \\ &\quad - 2 \left\langle (\nabla_s \vec{\eta})^T, \underline{\underline{D}}_s(\vec{\mathcal{V}}) (\nabla_s \vec{\text{id}})^T \right\rangle_{\Gamma(t)} \quad \forall \vec{\eta} \in \{\vec{\xi} \in [H^1(\Gamma_T)]^d : \partial_t^\circ \vec{\xi} = \vec{0}\}. \end{aligned} \quad (3.21)$$

On recalling (2.15), (2.12) and (2.8), we now consider the first variation of (2.14) subject to the side constraints

$$\langle \vec{\mathcal{K}}^\star, \vec{\eta} \rangle_{\Gamma(t)} + \left\langle \nabla_s \vec{\text{id}}, \nabla_s \vec{\eta} \right\rangle_{\Gamma(t)} = 0 \quad \forall \vec{\eta} \in [H^1(\Gamma(t))]^d, \quad (3.22a)$$

$$\left\langle \underline{\underline{w}}^\star, \underline{\underline{\zeta}} \right\rangle_{\Gamma(t)} + \frac{1}{2} \left\langle \vec{\nu}, [\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T] \vec{\mathcal{K}}^\star + \nabla_s \cdot [\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T] \right\rangle_{\Gamma(t)} = 0 \quad \forall \underline{\underline{\zeta}} \in [H^1(\Gamma(t))]^{d \times d}. \quad (3.22b)$$

Here we use the symmetric formulation in (3.22b), because its discretized form will then ensure that the discrete approximations to $\underline{\underline{w}}^\star$ are also symmetric, since

$$\left\langle (\underline{\underline{w}}^\star)^T, \underline{\underline{\zeta}} \right\rangle_{\Gamma(t)} = \left\langle \underline{\underline{w}}^\star, \underline{\underline{\zeta}}^T \right\rangle_{\Gamma(t)} = \left\langle \underline{\underline{w}}^\star, \underline{\underline{\zeta}} \right\rangle_{\Gamma(t)} \quad \forall \underline{\underline{\zeta}} \in [H^1(\Gamma(t))]^{d \times d}. \quad (3.23)$$

On recalling (2.14), we define the Lagrangian

$$\begin{aligned} L(\Gamma, \vec{\mathcal{K}}^\star, \vec{y}, \underline{\underline{w}}^\star, \underline{\underline{z}}, \mathbf{c}) &= \frac{1}{2} \left\langle \alpha(\mathbf{c}) |\vec{\mathcal{K}}^\star - \vec{\mathcal{K}}(\mathbf{c}) \vec{\nu}|^2, 1 \right\rangle_{\Gamma(t)} + \frac{1}{2} \left\langle \alpha^G(\mathbf{c}), |\vec{\mathcal{K}}^\star|^2 - |\underline{\underline{w}}^\star|^2 \right\rangle_{\Gamma(t)} \\ &\quad + \beta \left\langle b_{CH}(\mathbf{c}), 1 \right\rangle_{\Gamma(t)} - \left\langle \vec{\mathcal{K}}^\star, \vec{y} \right\rangle_{\Gamma(t)} - \left\langle \nabla_s \vec{\text{id}}, \nabla_s \vec{y} \right\rangle_{\Gamma(t)} \\ &\quad - \left\langle \underline{\underline{w}}^\star, \underline{\underline{z}} \right\rangle_{\Gamma(t)} - \frac{1}{2} \left\langle \vec{\nu}, [\underline{\underline{z}} + \underline{\underline{z}}^T] \vec{\mathcal{K}}^\star + \nabla_s \cdot [\underline{\underline{z}} + \underline{\underline{z}}^T] \right\rangle_{\Gamma(t)}, \end{aligned} \quad (3.24)$$

where $\vec{y} \in [H^1(\Gamma(t))]^d$ and $\underline{\underline{z}} \in [H^1(\Gamma(t))]^{d \times d}$ are Lagrange multipliers for (3.22a,b). In order to compute the direction of steepest descent, \vec{f}_Γ , of $E(\Gamma(t), \mathbf{c}(t))$, with respect to $\Gamma(t)$ and subject to the constraints (3.22a,b), we set the variations of $L(\Gamma, \vec{\mathcal{K}}^\star, \vec{y}, \underline{\underline{w}}^\star, \underline{\underline{z}}, \mathbf{c})$ with respect to $\vec{\mathcal{K}}^\star$, \vec{y} , $\underline{\underline{w}}^\star$ and $\underline{\underline{z}}$ to zero, and we use the variation with respect to \mathbf{c} to define the Cahn–Hilliard dynamics. Moreover, we obtain on using the formal calculus of

PDE constrained optimization, see e.g. Tröltzsch (2010), that

$$\left[\frac{\delta}{\delta \Gamma} L \right] (\vec{\chi}) = \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} [L(\Gamma_\varepsilon, \vec{\mathcal{Z}}_\varepsilon^*, \vec{y}_\varepsilon, \underline{\underline{w}}_\varepsilon^*, \underline{\underline{z}}_\varepsilon, \mathbf{c}_\varepsilon) - L(\Gamma, \vec{\mathcal{Z}}^*, \vec{y}, \underline{\underline{w}}^*, \underline{\underline{z}}, \mathbf{c})] = - \left\langle \vec{f}_\Gamma, \vec{\chi} \right\rangle_{\Gamma(t)}, \quad (3.25a)$$

$$\left[\frac{\delta}{\delta \vec{\mathcal{Z}}^*} L \right] (\vec{\xi}) = \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} [L(\Gamma, \vec{\mathcal{Z}}^* + \varepsilon \vec{\xi}, \vec{y}, \underline{\underline{w}}^*, \underline{\underline{z}}, \mathbf{c}) - L(\Gamma, \vec{\mathcal{Z}}^*, \vec{y}, \underline{\underline{w}}^*, \underline{\underline{z}}, \mathbf{c})] = 0, \quad (3.25b)$$

$$\left[\frac{\delta}{\delta \vec{y}} L \right] (\vec{\eta}) = \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} [L(\Gamma, \vec{\mathcal{Z}}^*, \vec{y} + \varepsilon \vec{\eta}, \underline{\underline{w}}^*, \underline{\underline{z}}, \mathbf{c}) - L(\Gamma, \vec{\mathcal{Z}}^*, \vec{y}, \underline{\underline{w}}^*, \underline{\underline{z}}, \mathbf{c})] = 0, \quad (3.25c)$$

$$\left[\frac{\delta}{\delta \underline{\underline{w}}^*} L \right] (\underline{\underline{\phi}}) = \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} [L(\Gamma, \vec{\mathcal{Z}}^*, \vec{y}, \underline{\underline{w}}^* + \varepsilon \underline{\underline{\phi}}, \underline{\underline{z}}, \mathbf{c}) - L(\Gamma, \vec{\mathcal{Z}}^*, \vec{y}, \underline{\underline{w}}^*, \underline{\underline{z}}, \mathbf{c})] = 0, \quad (3.25d)$$

$$\left[\frac{\delta}{\delta \underline{\underline{z}}} L \right] (\underline{\underline{\zeta}}) = \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} [L(\Gamma, \vec{\mathcal{Z}}^*, \vec{y}, \underline{\underline{w}}^*, \underline{\underline{z}} + \varepsilon \underline{\underline{\zeta}}, \mathbf{c}) - L(\Gamma, \vec{\mathcal{Z}}^*, \vec{y}, \underline{\underline{w}}^*, \underline{\underline{z}}, \mathbf{c})] = 0, \quad (3.25e)$$

$$\left[\frac{\delta}{\delta \mathbf{c}} L \right] (\xi) = \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} [L(\Gamma, \vec{\mathcal{Z}}^*, \vec{y}, \underline{\underline{w}}^*, \underline{\underline{z}}, \mathbf{c} + \varepsilon \xi) - L(\Gamma, \vec{\mathcal{Z}}^*, \vec{y}, \underline{\underline{w}}^*, \underline{\underline{z}}, \mathbf{c})] = \langle \mathbf{m}, \xi \rangle_{\Gamma(t)}, \quad (3.25f)$$

where $\vec{\mathcal{Z}}_\varepsilon^*, \vec{y}_\varepsilon \in [H^1(\Gamma_\varepsilon(t))]^d$, $\underline{\underline{w}}_\varepsilon^*, \underline{\underline{z}}_\varepsilon \in [H^1(\Gamma_\varepsilon(t))]^{d \times d}$, $\mathbf{c}_\varepsilon \in H^1(\Gamma_\varepsilon(t))$ are defined as in (3.11), and where \mathbf{m} defines the chemical potential. We note that (3.25c,e) immediately yield (3.22a,b), which means that we can recover $\vec{\mathcal{Z}}^*$ and $\underline{\underline{w}}^*$ in terms of $\Gamma(t)$ again. In particular, combining (2.13) and (3.22a) yields, on recalling (2.7) that $\vec{\mathcal{Z}}^* = \vec{\mathcal{Z}}$. In addition, it then follows from (3.22b) and (2.12) that $\underline{\underline{w}}^* = \underline{\underline{w}} = \nabla_s \vec{v}$. On recalling (1.2b), (3.12)–(3.15), (3.17) and (3.19) this yields that

$$\begin{aligned} & \left\langle \vec{f}_\Gamma, \vec{\chi} \right\rangle_{\Gamma(t)} - \langle \nabla_s \vec{y}, \nabla_s \vec{\chi} \rangle_{\Gamma(t)} - \langle \nabla_s \cdot \vec{y}, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} + 2 \left\langle (\nabla_s \vec{y})^T, \underline{\underline{D}}_s(\vec{\chi}) (\nabla_s \text{id})^T \right\rangle_{\Gamma(t)} \\ & + \frac{1}{2} \langle \alpha(\mathbf{c}) |\vec{\mathcal{Z}} - \overline{\mathcal{Z}}(\mathbf{c}) \vec{v}|^2 - 2 \vec{y} \cdot \vec{\mathcal{Z}}, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} + \langle \alpha(\mathbf{c}) \overline{\mathcal{Z}}(\mathbf{c}) (\vec{\mathcal{Z}} - \overline{\mathcal{Z}}(\mathbf{c}) \vec{v}), [\nabla_s \vec{\chi}]^T \vec{v} \rangle_{\Gamma(t)} \\ & + \beta \langle b_{CH}(\mathbf{c}), \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} - \beta \gamma \langle (\nabla_s \mathbf{c}) \otimes (\nabla_s \mathbf{c}), \nabla_s \vec{\chi} \rangle_{\Gamma(t)} \\ & + \frac{1}{2} \langle \alpha^G(\mathbf{c}) (|\vec{\mathcal{Z}}|^2 - |\underline{\underline{w}}|^2), \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} - \langle \underline{\underline{w}} : \underline{\underline{z}}, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} \\ & - \frac{1}{2} \langle \vec{v} \cdot ([\underline{\underline{z}} + \underline{\underline{z}}^T] \vec{\mathcal{Z}} + \nabla_s \cdot [\underline{\underline{z}} + \underline{\underline{z}}^T]), \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} - \sum_{i=1}^d \langle \nu_i \nabla_s \vec{z}_i, \nabla_s \vec{\chi} - 2 \underline{\underline{D}}_s(\vec{\chi}) \rangle_{\Gamma(t)} \\ & + \frac{1}{2} \langle [\underline{\underline{z}} + \underline{\underline{z}}^T] \vec{\mathcal{Z}} + \nabla_s \cdot [\underline{\underline{z}} + \underline{\underline{z}}^T], [\nabla_s \vec{\chi}]^T \vec{v} \rangle_{\Gamma(t)} = 0 \quad \forall \vec{\chi} \in [H^1(\Gamma(t))]^d, \end{aligned} \quad (3.26a)$$

$$\left\langle \alpha(\mathbf{c}) (\vec{\mathcal{Z}} - \overline{\mathcal{Z}}(\mathbf{c}) \vec{v}) + \alpha^G(\mathbf{c}) \vec{\mathcal{Z}} - \frac{1}{2} [\underline{\underline{z}} + \underline{\underline{z}}^T] \vec{v} - \vec{y}, \vec{\xi} \right\rangle_{\Gamma(t)} = 0 \quad \forall \vec{\xi} \in [H^1(\Gamma(t))]^d, \quad (3.26b)$$

$$\underline{\underline{z}} = -\alpha^G(\mathbf{c}) \underline{\underline{w}}, \quad (3.26c)$$

$$\langle \vec{\mathcal{Z}}, \vec{\eta} \rangle_{\Gamma(t)} + \left\langle \nabla_s \text{id}, \nabla_s \vec{\eta} \right\rangle_{\Gamma(t)} = 0 \quad \forall \vec{\eta} \in [H^1(\Gamma(t))]^d, \quad (3.26d)$$

$$\left\langle \underline{\underline{w}}, \underline{\underline{\zeta}} \right\rangle_{\Gamma(t)} + \frac{1}{2} \left\langle \vec{v}, [\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T] \vec{\mathcal{Z}} + \nabla_s \cdot [\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T] \right\rangle_{\Gamma(t)} = 0 \quad \forall \underline{\underline{\zeta}} \in [H^1(\Gamma(t))]^{d \times d}. \quad (3.26e)$$

The above is coupled to (3.4a–d) subject to the initial conditions (2.3). Here we have introduced $\vec{z}_i = \frac{1}{2} [\underline{z} + \underline{z}^T] \vec{e}_i$, $i = 1 \rightarrow d$, as well as $\nu_i = \vec{\nu} \cdot \vec{e}_i$, $i = 1 \rightarrow d$. Finally, on recalling (1.10a), and on using (2.13), (3.3), (3.2), (1.9) and (3.4c,d), a weak form of the Cahn–Hilliard dynamics is given by

$$\vartheta \frac{d}{dt} \langle \mathbf{c}, \eta \rangle_{\Gamma(t)} + \langle \nabla_s \mathbf{m}, \nabla_s \eta \rangle_{\Gamma(t)} = 0 \quad \forall \eta \in \{\xi \in H^1(\Gamma_T) : \partial_t^\circ \xi = 0\}, \quad (3.27a)$$

$$\begin{aligned} \langle \mathbf{m}, \xi \rangle_{\Gamma(t)} &= \beta \gamma \langle \nabla_s \mathbf{c}, \nabla_s \xi \rangle_{\Gamma(t)} + \beta \gamma^{-1} \langle \Psi'(\mathbf{c}), \xi \rangle_{\Gamma(t)} \\ &\quad + \frac{1}{2} \langle \alpha'(\mathbf{c}) |\vec{\mathcal{Z}} - \vec{\mathcal{Z}}(\mathbf{c}) \vec{\nu}|^2 - 2 \vec{\mathcal{Z}}'(\mathbf{c}) \alpha(\mathbf{c}) (\vec{\mathcal{Z}} - \vec{\mathcal{Z}}(\mathbf{c}) \vec{\nu}) \cdot \vec{\nu}, \xi \rangle_{\Gamma(t)} \\ &\quad + \frac{1}{2} \langle (\alpha^G)'(\mathbf{c}) (|\vec{\mathcal{Z}}|^2 - |\underline{w}|^2), \xi \rangle_{\Gamma(t)} \quad \forall \xi \in H^1(\Gamma(t)), \end{aligned} \quad (3.27b)$$

$$\mathbf{c}(\cdot, 0) = \mathbf{c}_0 \quad \text{on } \Gamma_0, \quad (3.27c)$$

with $\mathbf{c}_0 : \Gamma_0 \rightarrow \mathbb{R}$ given initial data, recall (2.3). Here we note that (3.27b) is well-posed for nonconstant α , α^G and $\vec{\mathcal{Z}}$ only in the case $\beta > 0$, which is why we assume that β is positive throughout the manuscript. In addition, we observe that choosing $\eta = 1$ in (3.27a) yields that

$$\frac{d}{dt} \langle \mathbf{c}, 1 \rangle_{\Gamma(t)} = 0. \quad (3.28)$$

REMARK. 3.2. *With regards to (3.26b) we note from (3.26c) and (2.8), as $\underline{w} = \nabla_s \vec{\nu} = (\nabla_s \vec{\nu})^T$, it holds that $\underline{z} = -\alpha^G(\mathbf{c}) \underline{w} = -\alpha^G(\mathbf{c}) \nabla_s \vec{\nu}$, and so $\underline{z} \vec{\nu} = \underline{z}^T \vec{\nu} = \vec{0}$. For further simplifications we refer to the appendix.*

We note the following LBB-type condition:

$$\inf_{(\varphi, \eta) \in \tilde{\mathbb{P}} \times L^2(\Gamma(t))} \sup_{\vec{\xi} \in \mathbb{U}_{\Gamma(t)}(\vec{0})} \frac{(\varphi, \nabla \cdot \vec{\xi}) + \langle \eta, \nabla_s \cdot \vec{\xi} \rangle_{\Gamma(t)}}{(\|\varphi\|_0 + \|\eta\|_{0, \Gamma(t)}) (\|\vec{\xi}\|_1 + \|\underline{\mathcal{P}}_\Gamma \vec{\xi}|_{\Gamma(t)}\|_{1, \Gamma(t)})} \geq C > 0, \quad (3.29)$$

which we also refer to as the LBB_Γ condition. Here we have defined the space $\mathbb{U}_{\Gamma(t)}(\vec{0}) := \{\vec{\xi} \in \mathbb{U}(\vec{0}) : \underline{\mathcal{P}}_\Gamma \vec{\xi}|_{\Gamma(t)} \in [H^1(\Gamma(t))]^d\}$, and let $\|\vec{\eta}\|_{1, \Gamma(t)}^2 := \langle \vec{\eta}, \vec{\eta} \rangle_{\Gamma(t)} + \langle \nabla_s \vec{\eta}, \nabla_s \vec{\eta} \rangle_{\Gamma(t)}$. In the case that the smooth hypersurface $\Gamma(t)$ is not a sphere, then (3.29) is shown to hold if $\partial_1 \Omega = \partial \Omega$ is a smooth boundary in Lengeler (2015, p. 15). See also the discussion around (2.11a,b) in Barrett et al. (2016a).

Overall the weak formulation for the free boundary problem (2.2a–d), (1.8), (1.5a–d), (1.6), (1.10a,b), (2.3), (3.27c) that we consider in this paper is given by

$$(P) \quad (3.4a\text{--}d), (3.26a\text{--}e), (3.27a\text{--}c), (2.3). \quad (3.30)$$

REMARK. 3.3. *We note that in the case $d = 2$ we do not consider Gaussian curvature terms, i.e. we assume that $\alpha^G(\mathbf{c}) = 0$. Then (3.26a) simplifies to*

$$\begin{aligned} &\left\langle \vec{f}_\Gamma, \vec{\chi} \right\rangle_{\Gamma(t)} - \langle \nabla_s \vec{y}, \nabla_s \vec{\chi} \rangle_{\Gamma(t)} - \langle \nabla_s \cdot \vec{y}, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} + 2 \left\langle (\nabla_s \vec{y})^T, \underline{D}_s(\vec{\chi}) (\nabla_s \text{id})^T \right\rangle_{\Gamma(t)} \\ &\quad + \frac{1}{2} \langle \alpha(\mathbf{c}) |\vec{\mathcal{Z}} - \vec{\mathcal{Z}}(\mathbf{c}) \vec{\nu}|^2 - 2 \vec{y} \cdot \vec{\mathcal{Z}}, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} + \langle \alpha(\mathbf{c}) \vec{\mathcal{Z}}(\mathbf{c}) (\vec{\mathcal{Z}} - \vec{\mathcal{Z}}(\mathbf{c}) \vec{\nu}), [\nabla_s \vec{\chi}]^T \vec{\nu} \rangle_{\Gamma(t)} \\ &\quad + \beta \langle b_{CH}(\mathbf{c}), \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} - \beta \gamma \langle (\partial_s \mathbf{c})^2, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} = 0 \quad \forall \vec{\chi} \in [H^1(\Gamma(t))]^d. \end{aligned} \quad (3.31)$$

Clearly, the last two terms in (3.31) can be absorbed by the surface pressure p_Γ in (3.4a). Hence, for constant α and constant $\overline{\alpha}$, the evolution of the interface is totally independent of the Cahn–Hilliard system. Of course, for $d = 3$ even for constant α , $\overline{\alpha}$ and α^G , the line tension term $\beta \gamma \langle (\nabla_s \mathbf{c}) \otimes (\nabla_s \mathbf{c}), \nabla_s \vec{\chi} \rangle_{\Gamma(t)}$ in (3.26a) means that nonconstant values of \mathbf{c} do have an influence on the membrane evolution.

4 Semidiscrete finite element approximation

For simplicity we consider Ω to be a polyhedral domain. Then let \mathcal{T}^h be a regular partitioning of Ω into disjoint open simplices o_j^h , $j = 1, \dots, J_\Omega$. Associated with \mathcal{T}^h are the finite element spaces

$$S_k^h := \{\chi \in C(\overline{\Omega}) : \chi|_o \in \mathcal{P}_k(o) \quad \forall o \in \mathcal{T}^h\} \subset H^1(\Omega), \quad k \in \mathbb{N},$$

where $\mathcal{P}_k(o)$ denotes the space of polynomials of degree k on o . We also introduce S_0^h , the space of piecewise constant functions on \mathcal{T}^h . Let $\{\varphi_{k,j}^h\}_{j=1}^{K_k^h}$ be the standard basis functions for S_k^h , $k \geq 0$. We introduce $\vec{I}_k^h : [C(\overline{\Omega})]^d \rightarrow [S_k^h]^d$, $k \geq 1$, the standard interpolation operators, such that $(\vec{I}_k^h \vec{\eta})(\vec{p}_{k,j}^h) = \vec{\eta}(\vec{p}_{k,j}^h)$ for $j = 1, \dots, K_k^h$; where $\{\vec{p}_{k,j}^h\}_{j=1}^{K_k^h}$ denotes the coordinates of the degrees of freedom of S_k^h , $k \geq 1$. In addition we define the standard projection operator $I_0^h : L^1(\Omega) \rightarrow S_0^h$, such that

$$(I_0^h \eta)|_o = \frac{1}{\mathcal{L}^d(o)} \int_o \eta \, d\mathcal{L}^d \quad \forall o \in \mathcal{T}^h.$$

Our approximation to the velocity and pressure on \mathcal{T}^h will be based on standard finite element spaces $\mathbb{U}^h(\vec{g}) \subset \mathbb{U}(\vec{I}_k^h \vec{g})$, for some $k \geq 2$, and $\mathbb{P}^h(t) \subset \mathbb{P}$, recall (3.1a,b). Here, for the former we assume from now on that $\vec{g} \in [C(\overline{\Omega})]^d$. We require also the space $\widehat{\mathbb{P}}^h(t) := \mathbb{P}^h(t) \cap \widehat{\mathbb{P}}$. Here, in general, we will choose pairs of velocity/pressure finite element spaces that satisfy the LBB inf-sup condition, see e.g. Girault and Raviart (1986, p. 114). For example, we may choose the lowest order Taylor-Hood element P2–P1 for $d = 2$ and $d = 3$, the P2–P0 element or the P2–(P1+P0) element for $d = 2$ on setting $\mathbb{U}^h(\vec{g}) = [S_2^h]^d \cap \mathbb{U}(\vec{I}_2^h \vec{g})$, and $\mathbb{P}^h = S_1^h$, S_0^h or $S_1^h + S_0^h$, respectively.

The parametric finite element spaces in order to approximate e.g. $\vec{\alpha}$ and \mathbf{c} are defined as follows. Similarly to Barrett et al. (2008), we introduce the following discrete spaces, based on the work of Dziuk (1991). Let $\Gamma^h(t) \subset \mathbb{R}^d$ be a $(d-1)$ -dimensional *polyhedral surface*, i.e. a union of non-degenerate $(d-1)$ -simplices with no hanging vertices (see Deckelnick et al. (2005, p. 164) for $d = 3$), approximating the closed surface $\Gamma(t)$. In particular, let $\Gamma^h(t) = \bigcup_{j=1}^{J_\Gamma} \overline{\sigma_j^h(t)}$, where $\{\sigma_j^h(t)\}_{j=1}^{J_\Gamma}$ is a family of mutually disjoint open $(d-1)$ -simplices with vertices $\{\vec{q}_k^h(t)\}_{k=1}^{K_\Gamma}$. Then let

$$\begin{aligned} W(\Gamma^h(t)) &:= \{\chi \in C(\Gamma^h(t)) : \chi|_{\sigma_j^h} \text{ is linear } \forall j = 1, \dots, J_\Gamma\}, \\ \underline{V}(\Gamma^h(t)) &:= \{\vec{\chi} \in [C(\Gamma^h(t))]^d : \vec{\chi}|_{\sigma_j^h} \text{ is linear } \forall j = 1, \dots, J_\Gamma\}, \\ \underline{\underline{V}}(\Gamma^h(t)) &:= \{\underline{\underline{\chi}} \in [C(\Gamma^h(t))]^{d \times d} : \underline{\underline{\chi}}|_{\sigma_j^h} \text{ is linear } \forall j = 1, \dots, J_\Gamma\}. \end{aligned}$$

Hence $W(\Gamma^h(t))$ is the space of scalar continuous piecewise linear functions on $\Gamma^h(t)$, with $\{\chi_k^h(\cdot, t)\}_{k=1}^{K_\Gamma}$ denoting the standard basis of $W(\Gamma^h(t))$, i.e.

$$\chi_k^h(\vec{q}_l^h(t), t) = \delta_{kl} \quad \forall k, l \in \{1, \dots, K_\Gamma\}, t \in [0, T]. \quad (4.1)$$

We require that $\Gamma^h(t) = \vec{X}^h(\Gamma^h(0), t)$ with $\vec{X}^h \in \underline{V}(\Gamma^h(0))$, and that $\vec{q}_k^h \in [H^1(0, T)]^d$, $k = 1, \dots, K_\Gamma$. For later purposes, we also introduce $\pi^h(t) : C(\Gamma^h(t)) \rightarrow W(\Gamma^h(t))$, the standard interpolation operator at the nodes $\{\vec{q}_k^h(t)\}_{k=1}^{K_\Gamma}$, and similarly $\bar{\pi}^h(t) : [C(\Gamma^h(t))]^d \rightarrow \underline{V}(\Gamma^h(t))$.

For scalar and vector functions η, ζ on $\Gamma^h(t)$ we introduce the L^2 -inner product $\langle \cdot, \cdot \rangle_{\Gamma^h(t)}$ over the polyhedral surface $\Gamma^h(t)$ as follows

$$\langle \eta, \zeta \rangle_{\Gamma^h(t)} := \int_{\Gamma^h(t)} \eta \cdot \zeta \, d\mathcal{H}^{d-1}.$$

In order to derive a stable numerical method, it is crucial to consider numerical integration in the discrete energy, see (4.13) below. Hence, for piecewise continuous functions v, w , with possible jumps across the edges of $\{\sigma_j^h(t)\}_{j=1}^{J_\Gamma}$, we introduce the mass lumped inner product $\langle \cdot, \cdot \rangle_{\Gamma^h(t)}^h$ as

$$\langle \eta, \phi \rangle_{\Gamma^h(t)}^h = \sum_{j=1}^J \langle \eta, \phi \rangle_{\sigma_j^h(t)}^h := \sum_{j=1}^J \frac{1}{d} \mathcal{H}^{d-1}(\sigma_j^h(t)) \sum_{k=1}^d (\eta \phi)((\vec{q}_{j_k}^h(t))^-), \quad (4.2)$$

where $\{\vec{q}_{j_k}^h(t)\}_{k=1}^d$ are the vertices of $\sigma_j^h(t)$, and where we define $\eta((\vec{q}_{j_k}^h(t))^-) := \lim_{\sigma_j^h(t) \ni \vec{p} \rightarrow \vec{q}_{j_k}^h(t)} \eta(\vec{p})$. We naturally extend this definition to vector and tensor functions.

Following Dziuk and Elliott (2013, (5.23)), we define the discrete material velocity for $\vec{z} \in \Gamma^h(t)$ by

$$\vec{\mathcal{V}}^h(\vec{z}, t) := \sum_{k=1}^{K_\Gamma} \left[\frac{d}{dt} \vec{q}_k^h(t) \right] \chi_k^h(\vec{z}, t). \quad (4.3)$$

For later use, we also introduce the finite element spaces

$$W_T(\Gamma_T^h) := \{\phi \in C(\Gamma_T^h) : \phi(\cdot, t) \in W(\Gamma^h(t)) \quad \forall t \in [0, T], \\ \phi(\vec{q}_k^h(t), t) \in H^1(0, T) \quad \forall k \in \{1, \dots, K\}\},$$

where $\Gamma_T^h := \bigcup_{t \in [0, T]} \Gamma^h(t) \times \{t\}$, as well as the vector- and tensor-valued analogues $\underline{V}_T(\Gamma_T^h)$ and $\underline{\underline{V}}_T(\Gamma_T^h)$. In a similar fashion, we introduce $W_T(\sigma_{j,T}^h)$ via

$$W_T(\sigma_{j,T}^h) := \{\phi \in C(\overline{\sigma_{j,T}^h}) : \phi(\cdot, t) \text{ is linear} \quad \forall t \in [0, T], \\ \phi(\vec{q}_{j_k}^h(t), t) \in H^1(0, T) \quad k = 1, \dots, d\},$$

where $\{\vec{q}_{j_k}^h(t)\}_{k=1}^d$ are the vertices of $\sigma_j^h(t)$, and where $\sigma_{j,T}^h := \bigcup_{t \in [0, T]} \sigma_j^h(t) \times \{t\}$, for $j \in \{1, \dots, J\}$.

Then, similarly to (3.2), we define the discrete material derivatives on $\Gamma^h(t)$ element-by-element via the equations

$$(\partial_t^{\circ,h} \phi)|_{\sigma_j^h(t)} = (\phi_t + \vec{\mathcal{V}}^h \cdot \nabla \phi)|_{\sigma_j^h(t)} \quad \forall \phi \in W_T(\sigma_{j,T}^h), \quad j \in \{1, \dots, J\}. \quad (4.4)$$

Moreover, similarly to (3.8), for any given $\vec{\chi} \in \underline{V}(\Gamma^h(t))$ we introduce

$$\Gamma_\varepsilon^h(t) := \{\vec{\Phi}^h(\vec{z}, \varepsilon) : \vec{z} \in \Gamma^h(t)\}, \quad \text{where} \quad \vec{\Phi}^h(\vec{z}, 0) = \vec{z} \quad \text{and} \quad \frac{\partial \vec{\Phi}^h}{\partial \varepsilon}(\vec{z}, 0) = \vec{\chi}(\vec{z}) \quad \forall \vec{z} \in \Gamma^h(t), \quad (4.5)$$

as well as $\partial_\varepsilon^{0,h}$ defined by (3.10) with $\Gamma(t)$ and $\vec{\Phi}$ replaced by $\Gamma^h(t)$ and $\vec{\Phi}^h$, respectively. We also introduce

$$\mathbb{V}_{\Gamma^h}^h(\vec{g}) := \{\vec{\phi} \in H^1(0, T; \mathbb{U}^h(\vec{g})) : \exists \vec{\chi} \in \underline{V}_T(\Gamma_T^h), \text{ s.t. } \vec{\chi}(\cdot, t) = \vec{\pi}^h[\vec{\phi}|_{\Gamma^h(t)}] \quad \forall t \in [0, T]\}. \quad (4.6)$$

On differentiating (4.1) with respect to t , it immediately follows that

$$\partial_t^{\circ,h} \chi_k^h = 0 \quad \forall k \in \{1, \dots, K_\Gamma\}, \quad (4.7)$$

see Dziuk and Elliott (2013, Lem. 5.5). It follows directly from (4.7) that

$$\partial_t^{\circ,h} \zeta(\cdot, t) = \sum_{k=1}^{K_\Gamma} \chi_k^h(\cdot, t) \frac{d}{dt} \zeta_k(t) \quad \text{on } \Gamma^h(t)$$

for $\zeta(\cdot, t) = \sum_{k=1}^{K_\Gamma} \zeta_k(t) \chi_k^h(\cdot, t) \in W(\Gamma^h(t))$, and hence $\partial_t^{\circ,h} \text{id} = \vec{\mathcal{V}}^h$ on $\Gamma^h(t)$.

We recall from Dziuk and Elliott (2013, Lem. 5.6) that

$$\frac{d}{dt} \int_{\sigma_j^h(t)} \zeta \, d\mathcal{H}^{d-1} = \int_{\sigma_j^h(t)} \partial_t^{\circ,h} \zeta + \zeta \nabla_s \cdot \vec{\mathcal{V}}^h \, d\mathcal{H}^{d-1} \quad \forall \zeta \in W_T(\sigma_{j,T}^h), \quad j \in \{1, \dots, J_\Gamma\}. \quad (4.8)$$

Moreover, on recalling (4.2), we have that

$$\begin{aligned} \frac{d}{dt} \langle \eta, \zeta \rangle_{\sigma_j^h(t)}^h &= \left\langle \partial_t^{\circ,h} \eta, \zeta \right\rangle_{\sigma_j^h(t)}^h + \left\langle \eta, \partial_t^{\circ,h} \zeta \right\rangle_{\sigma_j^h(t)}^h + \left\langle \eta \zeta, \nabla_s \cdot \vec{\mathcal{V}}^h \right\rangle_{\sigma_j^h(t)}^h \\ &\quad \forall \eta, \zeta \in W_T(\sigma_{j,T}^h), \quad j \in \{1, \dots, J_\Gamma\}. \end{aligned} \quad (4.9)$$

Given $\Gamma^h(t)$, we let $\Omega_+^h(t)$ denote the exterior of $\Gamma^h(t)$ and let $\Omega_-^h(t)$ denote the interior of $\Gamma^h(t)$, so that $\Gamma^h(t) = \partial\Omega_-^h(t) = \overline{\Omega_-^h(t)} \cap \overline{\Omega_+^h(t)}$. We then partition the elements of the bulk mesh \mathcal{T}^h into interior, exterior and interfacial elements as follows. Let

$$\begin{aligned} \mathcal{T}_-^h(t) &:= \{o \in \mathcal{T}^h : o \subset \Omega_-^h(t)\}, \\ \mathcal{T}_+^h(t) &:= \{o \in \mathcal{T}^h : o \subset \Omega_+^h(t)\}, \\ \mathcal{T}_{\Gamma^h}^h(t) &:= \{o \in \mathcal{T}^h : o \cap \Gamma^h(t) \neq \emptyset\}. \end{aligned}$$

Clearly $\mathcal{T}^h = \mathcal{T}_-^h(t) \cup \mathcal{T}_+^h(t) \cup \mathcal{T}_{\Gamma}^h(t)$ is a disjoint partition. In addition, we define the piecewise constant unit normal $\vec{\nu}^h(t)$ to $\Gamma^h(t)$ such that $\vec{\nu}^h(t)$ points into $\Omega_+^h(t)$. Moreover, we introduce the discrete density $\rho^h(t) \in S_0^h$ and the discrete viscosity $\mu^h(t) \in S_0^h$ as

$$\rho^h(t)|_o = \begin{cases} \rho_- & o \in \mathcal{T}_-^h(t), \\ \rho_+ & o \in \mathcal{T}_+^h(t), \\ \frac{1}{2}(\rho_- + \rho_+) & o \in \mathcal{T}_{\Gamma}^h(t), \end{cases} \quad \text{and} \quad \mu^h(t)|_o = \begin{cases} \mu_- & o \in \mathcal{T}_-^h(t), \\ \mu_+ & o \in \mathcal{T}_+^h(t), \\ \frac{1}{2}(\mu_- + \mu_+) & o \in \mathcal{T}_{\Gamma}^h(t). \end{cases}$$

Similarly to (1.7a,b), we introduce

$$\underline{\underline{\mathcal{P}}}_{\Gamma^h} = \underline{\underline{\text{Id}}} - \vec{\nu}^h \otimes \vec{\nu}^h \quad \text{on } \Gamma^h(t), \quad (4.10a)$$

and

$$\underline{\underline{D}}_s^h(\vec{\eta}) = \frac{1}{2} \underline{\underline{\mathcal{P}}}_{\Gamma^h} (\nabla_s \vec{\eta} + (\nabla_s \vec{\eta})^T) \underline{\underline{\mathcal{P}}}_{\Gamma^h} \quad \text{on } \Gamma^h(t), \quad (4.10b)$$

where here $\nabla_s = \underline{\underline{\mathcal{P}}}_{\Gamma^h} \nabla$ denotes the surface gradient on $\Gamma^h(t)$. Moreover, we introduce the vertex normal function $\vec{\omega}^h(\cdot, t) \in \underline{V}(\Gamma^h(t))$ with

$$\vec{\omega}^h(\vec{q}_k^h(t), t) := \frac{1}{\mathcal{H}^{d-1}(\Lambda_k^h(t))} \sum_{j \in \Theta_k^h} \mathcal{H}^{d-1}(\sigma_j^h(t)) \vec{\nu}^h|_{\sigma_j^h(t)}, \quad (4.11)$$

where for $k = 1, \dots, K_{\Gamma}^h$ we define $\Theta_k^h := \{j : \vec{q}_k^h(t) \in \overline{\sigma_j^h(t)}\}$ and set

$$\Lambda_k^h(t) := \cup_{j \in \Theta_k^h} \overline{\sigma_j^h(t)}.$$

For later use we note that

$$\langle \vec{z}, w \vec{\nu}^h \rangle_{\Gamma^h(t)}^h = \langle \vec{z}, w \vec{\omega}^h \rangle_{\Gamma^h(t)}^h \quad \forall \vec{z} \in \underline{V}(\Gamma^h(t)), w \in W(\Gamma^h(t)), \quad (4.12)$$

and so, in particular, $\langle \vec{z}, \vec{\nu}^h \rangle_{\Gamma^h(t)} = \langle \vec{z}, \vec{\nu}^h \rangle_{\Gamma^h(t)}^h = \langle \vec{z}, \vec{\omega}^h \rangle_{\Gamma^h(t)}^h$ for all $\vec{z} \in \underline{V}(\Gamma^h(t))$.

In what follows we will introduce a finite element approximation for the weak formulation (P), recall (3.30). By repeating on the discrete level the steps in §3.1, we will now derive a discrete analogue of (3.26a-e).

Similarly to the continuous setting in (2.14) and (3.22a,b), we consider the first variation of the discrete energy

$$\begin{aligned} E^h(\Gamma^h(t), \mathfrak{C}^h(t)) &= \frac{1}{2} \langle \alpha(\mathfrak{C}^h), |\vec{\kappa}^h - \vec{\mathcal{A}}(\mathfrak{C}^h) \vec{\nu}^h|^2 \rangle_{\Gamma^h(t)}^h + \frac{1}{2} \langle \alpha^G(\mathfrak{C}^h), |\vec{\kappa}^h|^2 - |\underline{\underline{W}}^h|^2 \rangle_{\Gamma^h(t)}^h \\ &\quad + \beta \langle b_{CH}(\mathfrak{C}^h), 1 \rangle_{\Gamma^h(t)}^h, \end{aligned} \quad (4.13)$$

where $\vec{\kappa}^h \in \underline{V}(\Gamma^h(t))$ and $\underline{\underline{W}}^h \in \underline{V}(\Gamma^h(t))$ have to satisfy side constraints

$$\langle \vec{\kappa}^h, \vec{\eta} \rangle_{\Gamma^h(t)}^h + \langle \nabla_s \vec{\text{id}}, \nabla_s \vec{\eta} \rangle_{\Gamma^h(t)}^h = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^h(t)), \quad (4.14a)$$

$$\langle \underline{\underline{W}}^h, \underline{\underline{\zeta}} \rangle_{\Gamma^h(t)}^h + \frac{1}{2} \langle \vec{\nu}^h, [\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T] \vec{\kappa}^h + \nabla_s \cdot [\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T] \rangle_{\Gamma^h(t)}^h = 0 \quad \forall \underline{\underline{\zeta}} \in \underline{V}(\Gamma^h(t)). \quad (4.14b)$$

Similarly to (3.24), we define the Lagrangian

$$\begin{aligned}
L^h(\Gamma^h, \bar{\kappa}^h, \bar{Y}^h, \underline{\underline{W}}^h, \underline{\underline{Z}}^h, \mathfrak{C}^h) \\
= \frac{1}{2} \langle \alpha(\mathfrak{C}^h), |\bar{\kappa}^h - \bar{\pi}(\mathfrak{C}^h)|^2 \rangle_{\Gamma^h(t)}^h + \frac{1}{2} \langle \alpha^G(\mathfrak{C}^h), |\bar{\kappa}^h|^2 - |\underline{\underline{W}}^h|^2 \rangle_{\Gamma^h(t)}^h \\
+ \beta \langle b_{CH}(\mathfrak{C}^h), 1 \rangle_{\Gamma^h(t)}^h - \langle \bar{\kappa}^h, \bar{Y}^h \rangle_{\Gamma^h(t)}^h - \langle \nabla_s \text{id}, \nabla_s \bar{Y}^h \rangle_{\Gamma^h(t)}^h \\
- \langle \underline{\underline{W}}^h, \underline{\underline{Z}}^h \rangle_{\Gamma^h(t)}^h - \frac{1}{2} \langle \bar{\nu}^h, [\underline{\underline{Z}}^h + (\underline{\underline{Z}}^h)^T] \bar{\kappa}^h + \nabla_s \cdot [\underline{\underline{Z}}^h + (\underline{\underline{Z}}^h)^T] \rangle_{\Gamma^h(t)}^h,
\end{aligned}$$

where $\bar{\kappa}^h \in \underline{V}(\Gamma^h(t))$, $\underline{\underline{W}}^h \in \underline{V}(\Gamma^h(t))$, $\mathfrak{C}^h \in W(\Gamma^h(t))$, with $\bar{Y}^h \in \underline{V}(\Gamma^h(t))$ and $\underline{\underline{Z}}^h \in \underline{V}(\Gamma^h(t))$ being Lagrange multipliers for (4.14a,b), respectively. Similarly to (3.26a–c), on recalling the formal calculus of PDE constrained optimization, we obtain the gradient $\bar{F}_\Gamma^h \in \underline{V}(\Gamma^h(t))$ of $E^h(\Gamma^h(t), \mathfrak{C}^h(t))$ with respect to $\Gamma^h(t)$ subject to the side constraints (4.14a,b) by setting $[\frac{\delta}{\delta \Gamma^h} L^h](\bar{\chi}) = - \langle \bar{F}_\Gamma^h, \bar{\chi} \rangle_{\Gamma^h(t)}^h$ for $\bar{\chi} \in \underline{V}(\Gamma^h(t))$, where we have recalled the definition (4.5), and by setting the remaining variations with respect to $\bar{\kappa}^h$, \bar{Y}^h , $\underline{\underline{W}}^h$ and $\underline{\underline{Z}}^h$ to zero. On noting (1.2b), (4.12) and the variation analogue of (4.9), as well as the obvious discrete variants of (3.12)–(3.15), (3.17) and (3.19), we then obtain that

$$\begin{aligned}
& \langle \bar{F}_\Gamma^h, \bar{\chi} \rangle_{\Gamma^h(t)}^h - \langle \nabla_s \bar{Y}^h, \nabla_s \bar{\chi} \rangle_{\Gamma^h(t)}^h - \langle \nabla_s \cdot \bar{Y}^h, \nabla_s \cdot \bar{\chi} \rangle_{\Gamma^h(t)}^h \\
& + \frac{1}{2} \langle \alpha(\mathfrak{C}^h), |\bar{\kappa}^h - \bar{\pi}(\mathfrak{C}^h)|^2 - 2 \bar{Y}^h \cdot \bar{\kappa}^h, \nabla_s \cdot \bar{\chi} \rangle_{\Gamma^h(t)}^h \\
& + 2 \langle (\nabla_s \bar{Y}^h)^T, \underline{\underline{D}}_s^h(\bar{\chi}) (\nabla_s \text{id})^T \rangle_{\Gamma^h(t)}^h + \langle \alpha(\mathfrak{C}^h) \bar{\pi}(\mathfrak{C}^h) (\bar{\kappa}^h - \bar{\pi}(\mathfrak{C}^h) \bar{\nu}^h), [\nabla_s \bar{\chi}]^T \bar{\nu}^h \rangle_{\Gamma^h(t)}^h \\
& + \beta \langle b_{CH}(\mathfrak{C}^h), \nabla_s \cdot \bar{\chi} \rangle_{\Gamma^h(t)}^h - \beta \gamma \langle (\nabla_s \mathfrak{C}^h) \otimes (\nabla_s \mathfrak{C}^h), \nabla_s \bar{\chi} \rangle_{\Gamma^h(t)}^h \\
& + \frac{1}{2} \langle \alpha^G(\mathfrak{C}^h) (|\bar{\kappa}^h|^2 - |\underline{\underline{W}}^h|^2), \nabla_s \cdot \bar{\chi} \rangle_{\Gamma^h(t)}^h - \langle \underline{\underline{W}}^h : \underline{\underline{Z}}^h, \nabla_s \cdot \bar{\chi} \rangle_{\Gamma^h(t)}^h \\
& - \frac{1}{2} \langle \bar{\nu}^h \cdot ([\underline{\underline{Z}}^h + (\underline{\underline{Z}}^h)^T] \bar{\kappa}^h + \nabla_s \cdot [\underline{\underline{Z}}^h + (\underline{\underline{Z}}^h)^T]), \nabla_s \cdot \bar{\chi} \rangle_{\Gamma^h(t)}^h \\
& - \sum_{i=1}^d \langle \nu_i^h \nabla_s \bar{Z}_i^h, \nabla_s \bar{\chi} - 2 \underline{\underline{D}}_s^h(\bar{\chi}) \rangle_{\Gamma^h(t)}^h \\
& + \frac{1}{2} \langle [\underline{\underline{Z}}^h + (\underline{\underline{Z}}^h)^T] \bar{\kappa}^h + \nabla_s \cdot [\underline{\underline{Z}}^h + (\underline{\underline{Z}}^h)^T], [\nabla_s \bar{\chi}]^T \bar{\nu}^h \rangle_{\Gamma^h(t)}^h = 0 \quad \forall \bar{\chi} \in \underline{V}(\Gamma^h(t)),
\end{aligned} \tag{4.15a}$$

$$\begin{aligned}
& \langle \alpha(\mathfrak{C}^h) (\bar{\kappa}^h - \bar{\pi}(\mathfrak{C}^h) \bar{\nu}^h) + \alpha^G(\mathfrak{C}^h) \bar{\kappa}^h - \frac{1}{2} [\underline{\underline{Z}}^h + (\underline{\underline{Z}}^h)^T] \bar{\nu}^h - \bar{Y}^h, \bar{\xi} \rangle_{\Gamma^h(t)}^h = 0 \\
& \quad \forall \bar{\xi} \in \underline{V}(\Gamma^h(t)),
\end{aligned} \tag{4.15b}$$

$$\underline{\underline{Z}}^h = \underline{\underline{\pi}}^h[-\alpha^G(\mathfrak{C}^h) \underline{\underline{W}}^h], \tag{4.15c}$$

as well as (4.14a,b) from the variations with respect to \bar{Y}^h and $\underline{\underline{Z}}^h$. Here we have introduced $\bar{Z}_i^h = \frac{1}{2} [\underline{\underline{Z}}^h + (\underline{\underline{Z}}^h)^T] \bar{e}_i$, $i = 1 \rightarrow d$, as well as $\nu_i^h = \bar{\nu}^h \cdot \bar{e}_i$, $i = 1 \rightarrow d$. Similarly to (3.23) it clearly follows from (4.14b) that

$$(\underline{\underline{W}}^h)^T = \underline{\underline{W}}^h \quad \Rightarrow \quad (\underline{\underline{Z}}^h)^T = \underline{\underline{Z}}^h, \tag{4.16}$$

and so many terms in (4.15a,b) can be simplified. We will perform these simplifications when we introduce the semidiscrete finite element approximation, see (4.18a–d), (4.19a–d) below. The Cahn–Hilliard dynamics are defined by

$$\vartheta \frac{d}{dt} \langle \mathfrak{C}^h, \chi_k^h \rangle_{\Gamma^h(t)}^h + \langle \nabla_s \mathfrak{M}^h, \nabla_s \chi_k^h \rangle_{\Gamma^h(t)} = 0 \quad \forall k \in \{1, \dots, K_\Gamma\}, \quad (4.17a)$$

$$\begin{aligned} \langle \mathfrak{M}^h, \xi \rangle_{\Gamma^h(t)}^h &= \beta \gamma \langle \nabla_s \mathfrak{C}^h, \nabla_s \xi \rangle_{\Gamma^h(t)} + \beta \gamma^{-1} \langle \Psi'(\mathfrak{C}^h), \xi \rangle_{\Gamma^h(t)}^h \\ &\quad + \frac{1}{2} \langle \alpha'(\mathfrak{C}^h) |\vec{\kappa}^h - \vec{\kappa}(\mathfrak{C}^h) \vec{\nu}^h|^2 - 2 \vec{\kappa}'(\mathfrak{C}^h) \alpha(\mathfrak{C}^h) (\vec{\kappa}^h - \vec{\kappa}(\mathfrak{C}^h) \vec{\nu}^h) \cdot \vec{\nu}^h, \xi \rangle_{\Gamma^h(t)}^h \\ &\quad + \frac{1}{2} \langle (\alpha^G)'(\mathfrak{C}^h) (|\vec{\kappa}^h|^2 - |\underline{\underline{W}}^h|^2), \xi \rangle_{\Gamma^h(t)}^h \quad \forall \xi \in W(\Gamma^h(t)), \end{aligned} \quad (4.17b)$$

where, similarly to the continuous setting (3.27a,b), we have defined $\mathfrak{M}^h \in W(\Gamma^h(t))$ by $\langle \mathfrak{M}^h, \xi \rangle_{\Gamma^h(t)}^h = [\frac{\delta}{\delta \mathfrak{C}^h} L^h](\xi)$ for all $\xi \in W(\Gamma^h(t))$.

Overall, we then obtain the following semidiscrete continuous-in-time finite element approximation, which is the semidiscrete analogue of the weak formulation (P), recall (3.30). Given $\Gamma^h(0)$, $\vec{U}^h(\cdot, 0) \in \mathbb{U}^h(\vec{g})$ and $\mathfrak{C}^h(\cdot, 0) \in W(\Gamma^h(0))$, find $(\Gamma^h(t))_{t \in (0, T]}$ such that $\text{id}|_{\Gamma^h(\cdot)} \in \underline{V}_T(\Gamma_T^h)$, with $\vec{\mathcal{V}}^h = \partial_t^{\circ, h} \text{id}|_{\Gamma^h(t)} \in \underline{V}(\Gamma^h(t))$ for all $t \in (0, T]$, and $\vec{U}^h \in \mathbb{V}_{\Gamma^h}^h(\vec{g})$, $\mathfrak{C}^h \in W_T(\Gamma_T^h)$, and, for all $t \in (0, T]$, $P^h(t) \in \widehat{\mathbb{P}}^h(t)$, $P_\Gamma^h(T) \in W(\Gamma^h(t))$, $\underline{\underline{W}}^h(t) \in \underline{\underline{V}}(\Gamma^h(t))$ and $\vec{\kappa}^h(t)$, $\vec{Y}^h(t)$, $\vec{F}_\Gamma^h(t) \in \underline{V}(\Gamma^h(t))$, $\mathfrak{M}^h \in W(\Gamma^h(t))$ such that (4.17a,b) holds, as well as

$$\begin{aligned} &\frac{1}{2} \left[\frac{d}{dt} \left(\rho^h \vec{U}^h, \vec{\xi} \right) + \left(\rho^h \vec{U}_t^h, \vec{\xi} \right) - \left(\rho^h \vec{U}^h, \vec{\xi}_t \right) + \rho_+ \left\langle \vec{U}^h \cdot \vec{n}, \vec{U}^h \cdot \vec{\xi} \right\rangle_{\partial_2 \Omega} \right] \\ &\quad + 2 \left(\mu^h \underline{\underline{D}}(\vec{U}^h), \underline{\underline{D}}(\vec{\xi}) \right) + \frac{1}{2} \left(\rho^h, [(\vec{U}^h \cdot \nabla) \vec{U}^h] \cdot \vec{\xi} - [(\vec{U}^h \cdot \nabla) \vec{\xi}] \cdot \vec{U}^h \right) - \left(P^h, \nabla \cdot \vec{\xi} \right) \\ &\quad + \rho_\Gamma \left\langle \partial_t^{\circ, h} \vec{\pi}^h \vec{U}^h, \vec{\xi} \right\rangle_{\Gamma^h(t)}^h + 2 \mu_\Gamma \left\langle \underline{\underline{D}}_s^h(\vec{\pi}^h \vec{U}^h), \underline{\underline{D}}_s^h(\vec{\pi}^h \vec{\xi}) \right\rangle_{\Gamma^h(t)} \\ &\quad - \left\langle P_\Gamma^h, \nabla_s \cdot (\vec{\pi}^h \vec{\xi}) \right\rangle_{\Gamma^h(t)} = \left(\rho^h \vec{f}^h, \vec{\xi} \right) + \left\langle \vec{F}_\Gamma^h, \vec{\xi} \right\rangle_{\Gamma^h(t)}^h \quad \forall \vec{\xi} \in H^1(0, T; \mathbb{U}^h(\vec{0})), \end{aligned} \quad (4.18a)$$

$$(\nabla \cdot \vec{U}^h, \varphi) = 0 \quad \forall \varphi \in \widehat{\mathbb{P}}^h(t), \quad (4.18b)$$

$$\left\langle \nabla_s \cdot (\vec{\pi}^h \vec{U}^h), \eta \right\rangle_{\Gamma^h(t)} = 0 \quad \forall \eta \in W(\Gamma^h(t)), \quad (4.18c)$$

$$\left\langle \vec{\mathcal{V}}^h, \vec{\chi} \right\rangle_{\Gamma^h(t)}^h = \left\langle \vec{U}^h, \vec{\chi} \right\rangle_{\Gamma^h(t)}^h \quad \forall \vec{\chi} \in \underline{V}(\Gamma^h(t)), \quad (4.18d)$$

where we recall (4.3), and

$$\langle \vec{\kappa}^h, \vec{\eta} \rangle_{\Gamma^h(t)}^h + \langle \nabla_s \text{id}, \nabla_s \vec{\eta} \rangle_{\Gamma^h(t)} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^h(t)), \quad (4.19a)$$

$$\langle \underline{W}^h, \underline{\zeta} \rangle_{\Gamma^h(t)}^h + \frac{1}{2} \langle \vec{\nu}^h, [\underline{\zeta} + \underline{\zeta}^T] \vec{\kappa}^h + \nabla_s \cdot [\underline{\zeta} + \underline{\zeta}^T] \rangle_{\Gamma^h(t)}^h = 0 \quad \forall \underline{\zeta} \in \underline{V}(\Gamma^h(t)), \quad (4.19b)$$

$$\langle \alpha(\mathfrak{E}^h) (\vec{\kappa}^h - \vec{\mathfrak{x}}(\mathfrak{E}^h) \vec{\nu}^h) + \alpha^G(\mathfrak{E}^h) (\vec{\mathfrak{x}} + \underline{W}^h \vec{\nu}^h) - \vec{Y}^h, \vec{\xi} \rangle_{\Gamma^h(t)}^h = 0 \quad \forall \vec{\xi} \in \underline{V}(\Gamma^h(t)), \quad (4.19c)$$

$$\begin{aligned} \langle \vec{F}_\Gamma^h, \vec{\chi} \rangle_{\Gamma^h(t)}^h &= \langle \nabla_s \vec{Y}^h, \nabla_s \vec{\chi} \rangle_{\Gamma^h(t)} + \langle \nabla_s \cdot \vec{Y}^h, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma^h(t)} \\ &\quad - \frac{1}{2} \langle [\alpha(\mathfrak{E}^h) |\vec{\kappa}^h - \vec{\mathfrak{x}}(\mathfrak{E}^h) \vec{\nu}^h|^2 - 2 \vec{Y}^h \cdot \vec{\kappa}^h], \nabla_s \cdot \vec{\chi} \rangle_{\Gamma^h(t)}^h \\ &\quad - 2 \langle (\nabla_s \vec{Y}^h)^T, \underline{D}_s^h(\vec{\chi}) (\nabla_s \text{id})^T \rangle_{\Gamma^h(t)} - \langle \alpha(\mathfrak{E}^h) \vec{\mathfrak{x}}(\mathfrak{E}^h) \vec{\kappa}^h, [\nabla_s \vec{\chi}]^T \vec{\nu}^h \rangle_{\Gamma^h(t)}^h \\ &\quad - \beta \langle b_{CH}(\mathfrak{E}^h), \nabla_s \cdot \vec{\chi} \rangle_{\Gamma^h(t)}^h + \beta \gamma \langle (\nabla_s \mathfrak{E}^h) \otimes (\nabla_s \mathfrak{E}^h), \nabla_s \vec{\chi} \rangle_{\Gamma^h(t)} \\ &\quad - \frac{1}{2} \langle \alpha^G(\mathfrak{E}^h) (|\vec{\kappa}^h|^2 + |\underline{W}^h|^2), \nabla_s \cdot \vec{\chi} \rangle_{\Gamma^h(t)}^h + \langle \vec{\nu}^h \cdot (\underline{Z}^h \vec{\kappa}^h + \nabla_s \cdot \underline{Z}^h), \nabla_s \cdot \vec{\chi} \rangle_{\Gamma^h(t)}^h \\ &\quad + \sum_{i=1}^d \langle \nu_i^h \nabla_s \vec{Z}_i^h, \nabla_s \vec{\chi} - 2 \underline{D}_s^h(\vec{\chi}) \rangle_{\Gamma^h(t)} - \langle \underline{Z}^h \vec{\kappa}^h + \nabla_s \cdot \underline{Z}^h, [\nabla_s \vec{\chi}]^T \vec{\nu}^h \rangle_{\Gamma^h(t)}^h \\ &\quad \forall \vec{\chi} \in \underline{V}(\Gamma^h(t)), \quad (4.19d) \end{aligned}$$

where $\underline{Z}^h = \underline{\pi}^h[-\alpha^G(\mathfrak{E}^h) \underline{W}^h]$ and $\vec{Z}_i^h = \underline{Z}^h \vec{e}_i$, $i = 1 \rightarrow d$. In addition, we have noted (4.16) and that $\alpha(\mathfrak{E}^h) \vec{\mathfrak{x}}^2(\mathfrak{E}^h) \vec{\nu}^h \cdot [\nabla_s \vec{\chi}]^T \vec{\nu}^h = 0$ on $\Gamma^h(t)$. Here we have defined $\vec{f}^h(\cdot, t) := \vec{I}_2^h \vec{f}(\cdot, t)$, where here and throughout we assume that $\vec{f} \in L^2(0, T; [C(\bar{\Omega})]^d)$. We note that in the special case of uniform α and $\vec{\mathfrak{x}}$, and if $\alpha^G = \beta = 0$, the scheme (4.18a–d), (4.19a–d) collapses to the semidiscrete approximation (4.15a–g), with $\beta = 0$, from Barrett et al. (2016b).

The following lemma is crucial in establishing a direct discrete analogue of (1.11).

LEMMA. 4.1. *Let $\{(\Gamma^h, \vec{U}^h, P^h, P_\Gamma^h, \vec{\kappa}^h, \vec{Y}^h, \vec{F}_\Gamma^h, \underline{W}^h, \underline{Z}^h, \mathfrak{E}^h, \mathfrak{M}^h)(t)\}_{t \in [0, T]}$ be a solution to (4.17a,b), (4.18a–d), (4.19a–d). In addition, we assume that $\vec{\kappa}^h \in \underline{V}_T(\Gamma_T^h)$ and $\underline{W}^h \in \underline{V}_T(\Gamma_T^h)$. Then*

$$\frac{d}{dt} E^h(\Gamma^h(t), \mathfrak{E}^h(t)) = - \langle \vec{F}_\Gamma^h, \vec{\nu}^h \rangle_{\Gamma^h(t)}^h + \langle \mathfrak{M}^h, \partial_t^{\circ, h} \mathfrak{E}^h \rangle_{\Gamma^h(t)}^h. \quad (4.20)$$

Proof. Taking the time derivatives of (4.14a,b), where we choose discrete test functions

$\vec{\eta}$ and $\underline{\underline{\zeta}}$ such that $\partial_t^{\circ,h} \vec{\eta} = \vec{0}$ and $\partial_t^{\circ,h} \underline{\underline{\zeta}} = \underline{\underline{0}}$, respectively, yields that

$$\begin{aligned} & \left\langle \partial_t^{\circ,h} \vec{\kappa}^h, \vec{\eta} \right\rangle_{\Gamma^h(t)}^h + \left\langle \vec{\kappa}^h \cdot \vec{\eta}, \nabla_s \cdot \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h + \left\langle \nabla_s \cdot \vec{\mathcal{V}}^h, \nabla_s \cdot \vec{\eta} \right\rangle_{\Gamma^h(t)} + \left\langle \nabla_s \cdot \vec{\mathcal{V}}^h, \nabla_s \cdot \vec{\eta} \right\rangle_{\Gamma^h(t)} \\ & - 2 \left\langle \underline{\underline{D}}_s^h(\vec{\mathcal{V}}^h) (\nabla_s \text{id})^T, (\nabla_s \vec{\eta})^T \right\rangle_{\Gamma^h(t)} = 0, \end{aligned} \quad (4.21a)$$

$$\begin{aligned} & \left\langle \partial_t^{\circ,h} \underline{\underline{W}}^h, \underline{\underline{\zeta}} \right\rangle_{\Gamma^h(t)}^h + \left\langle \underline{\underline{W}}^h : \underline{\underline{\zeta}}, \nabla_s \cdot \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h + \frac{1}{2} \left\langle \partial_t^{\circ,h} \vec{\nu}^h, [\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T] \vec{\kappa}^h + \nabla_s \cdot [\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T] \right\rangle_{\Gamma^h(t)}^h \\ & + \frac{1}{2} \left\langle \vec{\nu}^h \cdot ([\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T] \vec{\kappa}^h + \nabla_s \cdot [\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T]), \nabla_s \cdot \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h \\ & + \sum_{i=1}^d \left\langle \nu_i^h \nabla_s \vec{\zeta}_i, \nabla_s \vec{\mathcal{V}}^h - 2 \underline{\underline{D}}_s^h(\vec{\mathcal{V}}^h) \right\rangle_{\Gamma^h(t)} + \frac{1}{2} \left\langle \vec{\nu}^h, [\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T] \partial_t^{\circ,h} \vec{\kappa}^h \right\rangle_{\Gamma^h(t)}^h = 0, \end{aligned} \quad (4.21b)$$

where $\vec{\zeta}_i = \frac{1}{2} [\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T] \vec{e}_i$, $i = 1, \dots, d$. Here we have noted $\vec{\kappa}^h \in \underline{\underline{V}}_T(\Gamma_T^h)$, $\underline{\underline{W}}^h \in \underline{\underline{V}}_T(\Gamma_T^h)$, (4.9) and the discrete versions of (3.21) and (3.17). Choosing $\vec{\chi} = \vec{\mathcal{V}}^h$ in (4.15a), $\vec{\eta} = \vec{Y}^h$ in (4.21a) $\underline{\underline{\zeta}} = \underline{\underline{Z}}^h$ in (4.21b) and combining yields, on recalling (4.9) and the discrete

variants of (3.14) and (3.19), that

$$\begin{aligned}
& - \left\langle \vec{F}_\Gamma^h, \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h = \frac{1}{2} \left\langle \alpha(\mathfrak{E}^h) |\vec{\kappa}^h - \vec{\mathcal{K}}(\mathfrak{E}^h) \vec{\nu}^h|^2, \nabla_s \cdot \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h \\
& \quad - \left\langle \alpha(\mathfrak{E}^h) \vec{\mathcal{K}}(\mathfrak{E}^h) (\vec{\kappa}^h - \vec{\mathcal{K}}(\mathfrak{E}^h) \vec{\nu}^h), \partial_t^{\circ,h} \vec{\nu}^h \right\rangle_{\Gamma^h(t)}^h + \left\langle \partial_t^{\circ,h} \vec{\kappa}^h, \vec{Y}^h \right\rangle_{\Gamma^h(t)}^h \\
& \quad + \beta \left\langle b_{CH}(\mathfrak{E}^h), \nabla_s \cdot \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h - \beta \gamma \left\langle (\nabla_s \mathfrak{E}^h) \otimes (\nabla_s \mathfrak{E}^h), \nabla_s \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h \\
& \quad + \frac{1}{2} \left\langle \alpha^G(\mathfrak{E}^h) (|\vec{\kappa}^h|^2 - |\underline{\underline{W}}^h|^2), \nabla_s \cdot \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h + \left\langle \partial_t^{\circ,h} \underline{\underline{W}}^h, \underline{\underline{Z}}^h \right\rangle_{\Gamma^h(t)}^h \\
& \quad + \frac{1}{2} \left\langle \vec{\nu}^h, [\underline{\underline{Z}}^h + (\underline{\underline{Z}}^h)^T] \partial_t^{\circ,h} \vec{\kappa}^h \right\rangle_{\Gamma^h(t)}^h \\
& = \frac{1}{2} \left\langle \alpha(\mathfrak{E}^h) |\vec{\kappa}^h - \vec{\mathcal{K}}(\mathfrak{E}^h) \vec{\nu}^h|^2, \nabla_s \cdot \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h \\
& \quad - \left\langle \alpha(\mathfrak{E}^h) \vec{\mathcal{K}}(\mathfrak{E}^h) (\vec{\kappa}^h - \vec{\mathcal{K}}(\mathfrak{E}^h) \vec{\nu}^h), \partial_t^{\circ,h} \vec{\nu}^h \right\rangle_{\Gamma^h(t)}^h \\
& \quad + \left\langle \alpha(\mathfrak{E}^h) (\vec{\kappa}^h - \vec{\mathcal{K}}(\mathfrak{E}^h) \vec{\nu}^h) + \alpha^G(\mathfrak{E}^h) \vec{\kappa}^h, \partial_t^{\circ,h} \vec{\kappa}^h \right\rangle_{\Gamma^h(t)}^h \\
& \quad + \beta \left\langle b_{CH}(\mathfrak{E}^h), \nabla_s \cdot \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h - \beta \gamma \left\langle (\nabla_s \mathfrak{E}^h) \otimes (\nabla_s \mathfrak{E}^h), \nabla_s \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h \\
& \quad + \frac{1}{2} \left\langle \alpha^G(\mathfrak{E}^h) (|\vec{\kappa}^h|^2 - |\underline{\underline{W}}^h|^2), \nabla_s \cdot \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h - \left\langle \alpha^G(\mathfrak{E}^h) \partial_t^{\circ,h} \underline{\underline{W}}^h, \underline{\underline{W}}^h \right\rangle_{\Gamma^h(t)}^h \\
& = \frac{d}{dt} \left[\frac{1}{2} \left\langle \alpha(\mathfrak{E}^h), |\vec{\kappa}^h - \vec{\mathcal{K}}(\mathfrak{E}^h) \vec{\nu}^h|^2 \right\rangle_{\Gamma^h(t)}^h + \frac{1}{2} \left\langle \alpha^G(\mathfrak{E}^h), |\vec{\kappa}^h|^2 - |\underline{\underline{W}}^h|^2 \right\rangle_{\Gamma^h(t)}^h \right. \\
& \quad \left. + \beta \left\langle b_{CH}(\mathfrak{E}^h), 1 \right\rangle_{\Gamma^h(t)}^h \right] \\
& \quad - \frac{1}{2} \left\langle \alpha'(\mathfrak{E}^h) |\vec{\kappa}^h - \vec{\mathcal{K}}(\mathfrak{E}^h) \vec{\nu}^h|^2 - 2 \vec{\mathcal{K}}'(\mathfrak{E}^h) \alpha(\mathfrak{E}^h) (\vec{\kappa}^h - \vec{\mathcal{K}}(\mathfrak{E}^h) \vec{\nu}^h) \cdot \vec{\nu}^h, \partial_t^{\circ,h} \mathfrak{E}^h \right\rangle_{\Gamma^h(t)}^h \\
& \quad - \frac{1}{2} \left\langle (\alpha^G)'(\mathfrak{E}^h) (|\vec{\kappa}^h|^2 - |\underline{\underline{W}}^h|^2), \partial_t^{\circ,h} \mathfrak{E}^h \right\rangle_{\Gamma^h(t)}^h - \beta \gamma \left\langle \nabla_s \mathfrak{E}^h, \nabla_s \partial_t^{\circ,h} \mathfrak{E}^h \right\rangle_{\Gamma^h(t)}^h \\
& \quad - \beta \gamma^{-1} \left\langle \Psi'(\mathfrak{E}^h), \partial_t^{\circ,h} \mathfrak{E}^h \right\rangle_{\Gamma^h(t)}^h \\
& = \frac{d}{dt} E^h(\Gamma^h(t), \mathfrak{E}^h(t)) - \left\langle \mathfrak{M}^h, \partial_t^{\circ,h} \mathfrak{E}^h \right\rangle_{\Gamma^h(t)}^h \tag{4.22}
\end{aligned}$$

where we have noted (4.15b,c) and (4.17b), as well as $\mathfrak{E}^h \in W_T(\Gamma_T^h)$. This yields the desired result (4.20). \square

In the following theorem we derive discrete analogues of (1.11), (3.6) and (3.28) for the scheme (4.17a,b), (4.18a–d), (4.19a–d).

THEOREM. 4.2. *Let the assumptions of Lemma 4.1 hold. Then, in the case $\vec{g} = \vec{0}$, it*

holds that

$$\begin{aligned} & \frac{d}{dt} \left(\frac{1}{2} \|[\rho^h]^{\frac{1}{2}} \vec{U}^h\|_0^2 + \frac{1}{2} \rho_\Gamma \left\langle \vec{U}^h, \vec{U}^h \right\rangle_{\Gamma^h(t)}^h + E^h(\Gamma^h(t), \mathfrak{E}^h(t)) \right) + 2 \|[\mu^h]^{\frac{1}{2}} \underline{\underline{D}}(\vec{U}^h)\|_0^2 \\ & + 2 \mu_\Gamma \left\langle \underline{\underline{D}}_s^h(\vec{\pi}^h \vec{U}^h), \underline{\underline{D}}_s^h(\vec{\pi}^h \vec{U}^h) \right\rangle_{\Gamma^h(t)} + \frac{1}{2} \rho_+ \left\langle \vec{U}^h \cdot \vec{n}, |\vec{U}^h|^2 \right\rangle_{\partial_2 \Omega} \\ & + \vartheta^{-1} \left\langle \nabla_s \mathfrak{M}^h, \nabla_s \mathfrak{M}^h \right\rangle_{\Gamma^h(t)} = (\rho^h \vec{f}^h, \vec{U}^h). \end{aligned} \quad (4.23)$$

Moreover, it holds that

$$\frac{d}{dt} \langle \chi_k^h, 1 \rangle_{\Gamma^h(t)} = 0 \quad \forall k \in \{1, \dots, K_\Gamma\} \quad (4.24a)$$

and hence that

$$\frac{d}{dt} \mathcal{H}^{d-1}(\Gamma^h(t)) = 0. \quad (4.24b)$$

Finally, we have that

$$\frac{d}{dt} \langle \mathfrak{E}^h, 1 \rangle_{\Gamma^h(t)} = 0. \quad (4.24c)$$

Proof. Choosing $\vec{\xi} = \vec{U}^h$ in (4.18a), recall that $\vec{g} = \vec{0}$, $\varphi = P^h$ in (4.18b) and $\eta = P_\Gamma^h$ in (4.18c) yields that

$$\begin{aligned} & \frac{1}{2} \frac{d}{dt} \|[\rho^h]^{\frac{1}{2}} \vec{U}^h\|_0^2 + 2 \|[\mu^h]^{\frac{1}{2}} \underline{\underline{D}}(\vec{U}^h)\|_0^2 + \rho_\Gamma \left\langle \partial_t^{\circ, h} \vec{\pi}^h \vec{U}^h, \vec{U}^h \right\rangle_{\Gamma^h(t)}^h + \frac{1}{2} \rho_+ \left\langle \vec{U}^h \cdot \vec{n}, |\vec{U}^h|^2 \right\rangle_{\partial_2 \Omega} \\ & + 2 \mu_\Gamma \left\langle \underline{\underline{D}}_s^h(\vec{\pi}^h \vec{U}^h), \underline{\underline{D}}_s^h(\vec{\pi}^h \vec{U}^h) \right\rangle_{\Gamma^h(t)} = (\rho^h \vec{f}^h, \vec{U}^h) + \left\langle \vec{F}_\Gamma^h, \vec{U}^h \right\rangle_{\Gamma^h(t)}^h. \end{aligned} \quad (4.25)$$

Moreover, we note that (4.9), (4.18d) and (4.18c) with $\eta = \pi^h [|\vec{U}^h|_{\Gamma^h(t)}^2]$ imply that

$$\begin{aligned} \frac{1}{2} \rho_\Gamma \frac{d}{dt} \left\langle \vec{U}^h, \vec{U}^h \right\rangle_{\Gamma^h(t)}^h &= \frac{1}{2} \rho_\Gamma \left\langle \partial_t^{\circ, h} \vec{\pi}^h [|\vec{U}^h|^2], 1 \right\rangle_{\Gamma^h(t)}^h + \frac{1}{2} \rho_\Gamma \left\langle \nabla_s \cdot \vec{\mathcal{V}}^h, |\vec{U}^h|^2 \right\rangle_{\Gamma^h(t)}^h \\ &= \rho_\Gamma \left\langle \partial_t^{\circ, h} \vec{\pi}^h \vec{U}^h, \vec{U}^h \right\rangle_{\Gamma^h(t)}^h + \frac{1}{2} \rho_\Gamma \left\langle \nabla_s \cdot (\vec{\pi}^h \vec{U}^h), |\vec{\pi}^h \vec{U}^h|^2 \right\rangle_{\Gamma^h(t)}^h \\ &= \rho_\Gamma \left\langle \partial_t^{\circ, h} \vec{\pi}^h \vec{U}^h, \vec{U}^h \right\rangle_{\Gamma^h(t)}^h, \end{aligned} \quad (4.26)$$

where we have recalled $\vec{U}^h \in \mathbb{V}_{\Gamma^h}^h(\vec{g})$, see (4.6). Choosing $\vec{\chi} = \vec{F}_\Gamma^h$ in (4.18d), and combining with (4.20), yields that

$$\left\langle \vec{F}_\Gamma^h, \vec{U}^h \right\rangle_{\Gamma^h(t)}^h = \left\langle \vec{F}_\Gamma^h, \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h = -\frac{d}{dt} E^h(\Gamma^h(t), \mathfrak{E}^h(t)) + \left\langle \mathfrak{M}^h, \partial_t^{\circ, h} \mathfrak{E}^h \right\rangle_{\Gamma^h(t)}^h. \quad (4.27)$$

Moreover, similarly to (4.26), it follows from (4.9), (4.7) and (4.18c,d), on recalling $\mathfrak{E}^h \in W_T(\Gamma_T^h)$, that

$$\begin{aligned} \frac{d}{dt} \left\langle \mathfrak{E}^h, \chi_k^h \right\rangle_{\Gamma^h(t)}^h &= \left\langle \partial_t^{\circ, h} \mathfrak{E}^h, \chi_k^h \right\rangle_{\Gamma^h(t)}^h + \left\langle \mathfrak{E}^h \chi_k^h, \nabla_s \cdot \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h \\ &= \left\langle \partial_t^{\circ, h} \mathfrak{E}^h, \chi_k^h \right\rangle_{\Gamma^h(t)}^h + \left\langle \pi^h [\mathfrak{E}^h \chi_k^h], \nabla_s \cdot \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)}^h \\ &= \left\langle \partial_t^{\circ, h} \mathfrak{E}^h, \chi_k^h \right\rangle_{\Gamma^h(t)}^h + \left\langle \pi^h [\mathfrak{E}^h \chi_k^h], \nabla_s \cdot (\vec{\pi}^h \vec{U}^h) \right\rangle_{\Gamma^h(t)}^h = \left\langle \partial_t^{\circ, h} \mathfrak{E}^h, \chi_k^h \right\rangle_{\Gamma^h(t)}^h, \end{aligned} \quad (4.28)$$

for $k = 1, \dots, K_\Gamma$. Hence we obtain from (4.17a) that

$$-\left\langle \mathfrak{M}^h, \partial_t^{\circ, h} \mathfrak{C}^h \right\rangle_{\Gamma^h(t)}^h = \vartheta^{-1} \left\langle \nabla_s \mathfrak{M}^h, \nabla_s \mathfrak{M}^h \right\rangle_{\Gamma^h(t)}. \quad (4.29)$$

The desired result (4.23) now directly follows from combining (4.25), (4.26), (4.27) and (4.29).

Similarly to (3.6), it immediately follows from (4.8) and (4.7), on choosing $\eta = \chi_k^h$ in (4.18c), and on recalling from (4.18d) that $\vec{\mathcal{V}}^h = \vec{\pi}^h [\vec{U}^h|_{\Gamma^h(t)}]$, that

$$\frac{d}{dt} \left\langle \chi_k^h, 1 \right\rangle_{\Gamma^h(t)} = \left\langle \chi_k^h, \nabla_s \cdot \vec{\mathcal{V}}^h \right\rangle_{\Gamma^h(t)} = 0, \quad (4.30)$$

which proves the desired result (4.24a). Summing (4.24a) for all $k = 1, \dots, K_\Gamma$ then yields the desired result (4.24b). Similarly, summing (4.17a) for $k = 1, \dots, K_\Gamma$ yields the desired result (4.24c). \square

We observe that it does not appear possible to prove a discrete analogue of (3.7) for the scheme (4.17a,b), (4.18a–d), (4.19a–d), even if the pressure space $\mathbb{P}^h(t)$ is enriched by the characteristic function of the inner phase, $\mathcal{X}_{\Omega_-^h(t)}$. Following the approach introduced in Barrett et al. (2016a,b), we enforce

$$\left\langle \vec{U}^h, \vec{\omega}^h \right\rangle_{\Gamma^h(t)}^h = 0, \quad (4.31)$$

which will lead to volume conservation for the two phases on the discrete level. As (4.31) cannot be interpreted in terms of enriching $\mathbb{P}^h(t)$, we enforce it separately with the help of a Lagrange multiplier, which we denote by P_{sing}^h . We are now in a position to propose the following adaptation of (4.17a,b), (4.18a–d), (4.19a–d)

Given $\Gamma^h(0)$, $\vec{U}^h(\cdot, 0) \in \mathbb{U}^h(\vec{g})$ and $\mathfrak{C}^h(\cdot, 0) \in W(\Gamma^h(0))$, find $(\Gamma^h(t))_{t \in (0, T]}$ such that $\text{id}|_{\Gamma^h(\cdot)} \in \underline{V}_T(\Gamma_T^h)$, with $\vec{\mathcal{V}}^h = \partial_t^{\circ, h} \text{id}|_{\Gamma^h(t)} \in \underline{V}(\Gamma^h(t))$ for all $t \in (0, T]$, and $\vec{U}^h \in \mathbb{V}_{\Gamma^h}^h(\vec{g})$, $\mathfrak{C}^h \in W_T(\Gamma_T^h)$, and, for all $t \in (0, T]$, $P^h(t) \in \widehat{\mathbb{P}}^h(t)$, $P_{\text{sing}}^h(t) \in \mathbb{R}$, $P_\Gamma^h(t) \in W(\Gamma^h(t))$, $\underline{W}^h(t) \in \underline{V}(\Gamma^h(t))$ and $\vec{\kappa}^h(t)$, $\vec{Y}^h(t)$, $\vec{F}_\Gamma^h(t) \in \underline{V}(\Gamma^h(t))$, $\mathfrak{M}^h \in W(\Gamma^h(t))$ such that (4.17a,b) holds, as well as

$$\begin{aligned} & \frac{1}{2} \left[\frac{d}{dt} \left(\rho^h \vec{U}^h, \vec{\xi} \right) + \left(\rho^h \vec{U}_t^h, \vec{\xi} \right) - \left(\rho^h \vec{U}^h, \vec{\xi}_t \right) + \rho_+ \left\langle \vec{U}^h \cdot \vec{n}, \vec{U}^h \cdot \vec{\xi} \right\rangle_{\partial_2 \Omega} \right] \\ & + 2 \left(\mu^h \underline{D}(\vec{U}^h), \underline{D}(\vec{\xi}) \right) + \frac{1}{2} \left(\rho^h, [(\vec{U}^h \cdot \nabla) \vec{U}^h] \cdot \vec{\xi} - [(\vec{U}^h \cdot \nabla) \vec{\xi}] \cdot \vec{U}^h \right) - \left(P^h, \nabla \cdot \vec{\xi} \right) \\ & - P_{\text{sing}}^h \left\langle \vec{\omega}^h, \vec{\xi} \right\rangle_{\Gamma^h(t)}^h + \rho_\Gamma \left\langle \partial_t^{\circ, h} \vec{\pi}^h \vec{U}^h, \vec{\xi} \right\rangle_{\Gamma^h(t)}^h + 2 \mu_\Gamma \left\langle \underline{D}_s^h(\vec{\pi}^h \vec{U}^h), \underline{D}_s^h(\vec{\pi}^h \vec{\xi}) \right\rangle_{\Gamma^h(t)} \\ & - \left\langle P_\Gamma^h, \nabla_s \cdot (\vec{\pi}^h \vec{\xi}) \right\rangle_{\Gamma^h(t)} = \left(\rho^h \vec{f}^h, \vec{\xi} \right) + \left\langle \vec{F}_\Gamma^h, \vec{\xi} \right\rangle_{\Gamma^h(t)}^h \quad \forall \vec{\xi} \in H^1(0, T; \mathbb{U}^h(\vec{0})), \end{aligned} \quad (4.32a)$$

$$\left(\nabla \cdot \vec{U}^h, \varphi \right) = 0 \quad \forall \varphi \in \widehat{\mathbb{P}}^h(t) \quad \text{and} \quad \left\langle \vec{U}^h, \vec{\omega}^h \right\rangle_{\Gamma^h(t)}^h = 0 \quad (4.32b)$$

and (4.18c,d), (4.19a–d) hold. We now have the following result.

THEOREM. 4.3. Let $\{(\Gamma^h, \vec{U}^h, P^h, P_{\text{sing}}^h, P_\Gamma^h, \vec{\kappa}^h, \vec{Y}^h, \vec{F}_\Gamma^h, \underline{W}^h, \underline{Z}^h, \mathfrak{C}^h, \mathfrak{M}^h)(t)\}_{t \in [0, T]}$ be a solution to (4.17a,b), (4.32a,b), (4.18c,d), (4.19a-d). In addition, we assume that $\vec{\kappa}^h \in \underline{V}_T(\Gamma_T^h)$ and $\underline{W}^h \in \underline{V}_T(\Gamma_T^h)$. Then (4.23) holds if $\vec{g} = \vec{0}$. In addition, (4.24a-c) and

$$\frac{d}{dt} \mathcal{L}^d(\Omega_-^h(t)) = 0 \quad (4.33)$$

hold.

Proof. The proofs for (4.23) and (4.24a-c) are analogous to the proofs in Theorem 4.2. In order to prove (4.33) we choose $\vec{\chi} = \vec{\omega}^h \in \underline{V}(\Gamma^h(t))$ in (4.18d) to yield that

$$\frac{d}{dt} \mathcal{L}^d(\Omega_-^h(t)) = \left\langle \vec{\mathcal{V}}^h, \vec{\nu}^h \right\rangle_{\Gamma^h(t)} = \left\langle \vec{\mathcal{V}}^h, \vec{\nu}^h \right\rangle_{\Gamma^h(t)}^h = \left\langle \vec{\mathcal{V}}^h, \vec{\omega}^h \right\rangle_{\Gamma^h(t)}^h = \left\langle \vec{U}^h, \vec{\omega}^h \right\rangle_{\Gamma^h(t)}^h = 0,$$

where we have used Deckelnick et al. (2005, Lemma 2.1), (4.12) and (4.32b). \square

5 Fully discrete finite element approximation

We consider the partitioning $t_m = m\tau$, $m = 0, \dots, M$, of $[0, T]$ into uniform time steps $\tau = T/M$. The time discrete spatial discretizations then directly follow from the finite element spaces introduced in §4, where in order to allow for adaptivity in space we consider bulk finite element spaces that change in time. For all $m \geq 0$, let \mathcal{T}^m be a regular partitioning of Ω into disjoint open simplices σ_j^m , $j = 1, \dots, J_\Omega^m$. Associated with \mathcal{T}^m are the finite element spaces $S_k^m(\Omega)$ for $k \geq 0$. We introduce also $\vec{I}_k^m : [C(\bar{\Omega})]^d \rightarrow [S_k^m(\Omega)]^d$, $k \geq 1$, the standard interpolation operators, and the standard projection operator $I_0^m : L^1(\Omega) \rightarrow S_0^m(\Omega)$. The parametric finite element spaces are given by

$$\underline{V}(\Gamma^m) := \{\vec{\chi} \in [C(\Gamma^m)]^d : \vec{\chi}|_{\sigma_j^m} \text{ is linear } \forall j = 1, \dots, J_\Gamma\} =: [W(\Gamma^m)]^d,$$

for $m = 0, \dots, M-1$, and similarly for $\underline{V}(\Gamma^m)$. Here $\Gamma^m = \bigcup_{j=1}^{J_\Gamma} \bar{\sigma}_j^m$, where $\{\sigma_j^m\}_{j=1}^{J_\Gamma}$ is a family of mutually disjoint open $(d-1)$ -simplices with vertices $\{\vec{q}_k^m\}_{k=1}^{K_\Gamma}$. We denote the standard basis of $W(\Gamma^m)$ by $\{\chi_k^m(\cdot, t)\}_{k=1}^{K_\Gamma}$. We also introduce $\pi^m : C(\Gamma^m) \rightarrow W(\Gamma^m)$, the standard interpolation operator at the nodes $\{\vec{q}_k^m\}_{k=1}^{K_\Gamma}$, and similarly $\vec{\pi}^m : [C(\Gamma^m)]^d \rightarrow \underline{V}(\Gamma^m)$. Throughout this paper, we will parameterize the new closed surface Γ^{m+1} over Γ^m , with the help of a parameterization $\vec{X}^{m+1} \in \underline{V}(\Gamma^m)$, i.e. $\Gamma^{m+1} = \vec{X}^{m+1}(\Gamma^m)$. Moreover, let

$$W_{\leq 1}(\Gamma^m) := \{\chi \in W(\Gamma^m) : |\chi| \leq 1\}. \quad (5.1)$$

Given Γ^m , we let Ω_+^m denote the exterior of Γ^m and let Ω_-^m denote the interior of Γ^m , so that $\Gamma^m = \partial\Omega_-^m = \bar{\Omega}_-^m \cap \bar{\Omega}_+^m$. In addition, we define the piecewise constant unit normal $\vec{\nu}^m$ to Γ^m such that $\vec{\nu}^m$ points into Ω_+^m . We then partition the elements of the

bulk mesh \mathcal{T}^m into interior, exterior and interfacial elements as before, and we introduce $\rho^m, \mu^m \in S_0^m(\Omega)$, for $m \geq 0$, as

$$\rho^m|_{o^m} = \begin{cases} \rho_- & o^m \in \mathcal{T}_-^m, \\ \rho_+ & o^m \in \mathcal{T}_+^m, \\ \frac{1}{2}(\rho_- + \rho_+) & o^m \in \mathcal{T}_{\Gamma^m}^m, \end{cases} \quad \text{and} \quad \mu^m|_{o^m} = \begin{cases} \mu_- & o^m \in \mathcal{T}_-^m, \\ \mu_+ & o^m \in \mathcal{T}_+^m, \\ \frac{1}{2}(\mu_- + \mu_+) & o^m \in \mathcal{T}_{\Gamma^m}^m. \end{cases}$$

We also introduce the L^2 -inner product $\langle \cdot, \cdot \rangle_{\Gamma^m}$ over the current polyhedral surface Γ^m , as well as the mass lumped inner product $\langle \cdot, \cdot \rangle_{\Gamma^m}^h$. We introduce, similarly to (4.10a,b),

$$\underline{\mathcal{P}}_{\Gamma^m} = \underline{\text{Id}} - \vec{\nu}^m \otimes \vec{\nu}^m \quad \text{on } \Gamma^m,$$

and

$$\underline{\underline{D}}_s^m(\vec{\eta}) = \frac{1}{2} \underline{\mathcal{P}}_{\Gamma^m} (\nabla_s \vec{\eta} + (\nabla_s \vec{\eta})^T) \underline{\mathcal{P}}_{\Gamma^m} \quad \text{on } \Gamma^m,$$

where here $\nabla_s = \underline{\mathcal{P}}_{\Gamma^m} \nabla$ denotes the surface gradient on Γ^m .

We introduce the following pushforward operator for the discrete interfaces Γ^m and Γ^{m-1} , for $m = 0, \dots, M$. Here we set $\Gamma^{-1} := \Gamma^0$. Let $\vec{\Pi}_{m-1}^m : [C(\Gamma^{m-1})]^d \rightarrow \underline{V}(\Gamma^m)$ such that

$$(\vec{\Pi}_{m-1}^m \vec{z})(\vec{q}_k^m) = \vec{z}(\vec{q}_k^{m-1}), \quad k = 1, \dots, K_\Gamma, \quad \forall \vec{z} \in [C(\Gamma^{m-1})]^d, \quad (5.2)$$

for $m = 1, \dots, M$, and set $\vec{\Pi}_{-1}^0 := \vec{\pi}^0$. Analogously to (5.2) we also introduce $\Pi_{m-1}^m : C(\Gamma^{m-1}) \rightarrow W(\Gamma^m)$ and $\underline{\underline{\Pi}}_{m-1}^m : [C(\Gamma^{m-1})]^{d \times d} \rightarrow \underline{\underline{V}}(\Gamma^m)$. We also introduce the short hand notations

$$\alpha^m = \pi^m[\alpha(\mathfrak{C}^m)], \quad \mathfrak{x}^m = \pi^m[\mathfrak{x}(\mathfrak{C}^m)], \quad \alpha^{G,m} = \pi^m[\alpha^G(\mathfrak{C}^m)], \quad (5.3)$$

for $m = 0, \dots, M-1$. We note, similarly to (4.12), that

$$\langle \vec{z}, w \vec{\nu}^m \rangle_{\Gamma^m}^h = \langle \vec{z}, w \vec{\omega}^m \rangle_{\Gamma^m}^h \quad \forall \vec{z} \in \underline{V}(\Gamma^m), \quad w \in W(\Gamma^m),$$

where $\vec{\omega}^m := \sum_{k=1}^{K_\Gamma} \chi_k^m \vec{\omega}_k^m \in \underline{V}(\Gamma^m)$, and where for $k = 1, \dots, K_\Gamma$ we let $\Theta_k^m := \{j : \vec{q}_k^m \in \overline{\sigma_j^m}\}$ and set $\Lambda_k^m := \cup_{j \in \Theta_k^m} \overline{\sigma_j^m}$ and $\vec{\omega}_k^m := \frac{1}{\mathcal{H}^{d-1}(\Lambda_k^m)} \sum_{j \in \Theta_k^m} \mathcal{H}^{d-1}(\sigma_j^m) \vec{\nu}_j^m$.

For the approximation to the velocity and pressure on \mathcal{T}^m we use the finite element spaces $\mathbb{U}^m(\vec{g})$ and \mathbb{P}^m , which are the direct time discrete analogues of $\mathbb{U}^h(\vec{g})$ and $\mathbb{P}^h(t_m)$, as well as $\widehat{\mathbb{P}}^m \subset \widehat{\mathbb{P}}$.

Analogously to (3.29), we recall the following discrete LBB $_\Gamma$ inf-sup assumption from Barrett et al. (2016b). Let there exist a $C_0 \in \mathbb{R}_{>0}$, independent of \mathcal{T}^m and $\{\sigma_j^m\}_{j=1}^{J_\Gamma}$, such that

$$\inf_{(\varphi, \lambda, \eta) \in \widehat{\mathbb{P}}^m \times \mathbb{R} \times W(\Gamma^m)} \sup_{\vec{\xi} \in \mathbb{U}^m(\vec{0})} \frac{(\varphi, \nabla \cdot \vec{\xi}) + \lambda \left\langle \vec{\omega}^m, \vec{\xi} \right\rangle_{\Gamma^m}^h + \left\langle \eta, \nabla_s \cdot (\vec{\pi}^m \vec{\xi}|_{\Gamma^m}) \right\rangle_{\Gamma^m}}{(\|\varphi\|_0 + |\lambda| + \|\eta\|_{0, \Gamma^m}) (\|\vec{\xi}\|_1 + \|\underline{\mathcal{P}}_{\Gamma^m}(\vec{\pi}^m \vec{\xi}|_{\Gamma^m})\|_{1, \Gamma^m, h})} \geq C_0, \quad (5.4)$$

where $\|\eta\|_{0,\Gamma^m}^2 := \langle \eta, \eta \rangle_{\Gamma^m}$ and $\|\vec{\eta}\|_{1,\Gamma^m,h}^2 := \langle \vec{\eta}, \vec{\eta} \rangle_{\Gamma^m} + \sum_{j=1}^{J_\Gamma} \int_{\sigma_j^m} |\nabla_s \vec{\eta}|^2 d\mathcal{H}^{d-1}$. See Barrett et al. (2016b, (5.2)) for more details.

Our proposed fully discrete approximation is given as follows. Let Γ^0 , an approximation to $\Gamma(0)$, as well as $\vec{\kappa}^0 \in \underline{V}(\Gamma^0)$, $\mathfrak{C}^0 \in W(\Gamma^0)$ and $\vec{U}^0 \in \mathbb{U}^0(\vec{g})$ be given. For $m = 0, \dots, M-1$, find $\vec{U}^{m+1} \in \mathbb{U}^m(\vec{g})$, $P^{m+1} \in \widehat{\mathbb{P}}^m$, $P_{\text{sing}}^{m+1} \in \mathbb{R}$, $P_\Gamma^{m+1} \in W(\Gamma^m)$, $\vec{X}^{m+1} \in \underline{V}(\Gamma^m)$, $\vec{\kappa}^{m+1} \in \underline{V}(\Gamma^m)$, $\underline{W}^{m+1} \in \underline{V}(\Gamma^m)$ and $\vec{Y}^{m+1}, \vec{F}_\Gamma^{m+1} \in \underline{V}(\Gamma^m)$ such that

$$\begin{aligned} & \frac{1}{2} \left(\frac{\rho^m \vec{U}^{m+1} - (I_0^m \rho^{m-1}) \vec{I}_2^m \vec{U}^m}{\tau} + (I_0^m \rho^{m-1}) \frac{\vec{U}^{m+1} - \vec{I}_2^m \vec{U}^m}{\tau}, \vec{\xi} \right) \\ & + 2 \left(\mu^m \underline{D}(\vec{U}^{m+1}), \underline{D}(\vec{\xi}) \right) + \frac{1}{2} \left(\rho^m, [(\vec{I}_2^m \vec{U}^m \cdot \nabla) \vec{U}^{m+1}] \cdot \vec{\xi} - [(\vec{I}_2^m \vec{U}^m \cdot \nabla) \vec{\xi}] \cdot \vec{U}^{m+1} \right) \\ & - \left(P^{m+1}, \nabla \cdot \vec{\xi} \right) - P_{\text{sing}}^{m+1} \left\langle \vec{\omega}^m, \vec{\xi} \right\rangle_{\Gamma^m}^h + \rho_\Gamma \left\langle \frac{\vec{U}^{m+1} - \vec{\Pi}_{m-1}^m (\vec{I}_2^m \vec{U}^m)|_{\Gamma^{m-1}}}{\tau}, \vec{\xi} \right\rangle_{\Gamma^m}^h \\ & + 2 \mu_\Gamma \left\langle \underline{D}_s^m(\vec{\pi}^m \vec{U}^{m+1}), \underline{D}_s^m(\vec{\pi}^m \vec{\xi}) \right\rangle_{\Gamma^m} - \left\langle P_\Gamma^{m+1}, \nabla_s \cdot (\vec{\pi}^m \vec{\xi}) \right\rangle_{\Gamma^m} \\ & = \left(\rho^m \vec{f}^{m+1}, \vec{\xi} \right) + \left\langle \vec{F}_\Gamma^{m+1}, \vec{\xi} \right\rangle_{\Gamma^m}^h - \frac{1}{2} \rho_+ \left\langle \vec{U}^m \cdot \vec{n}, \vec{U}^m \cdot \vec{\xi} \right\rangle_{\partial_2 \Omega} \quad \forall \vec{\xi} \in \mathbb{U}^m(\vec{0}), \end{aligned} \tag{5.5a}$$

$$\left(\nabla \cdot \vec{U}^{m+1}, \varphi \right) = 0 \quad \forall \varphi \in \widehat{\mathbb{P}}^m \quad \text{and} \quad \left\langle \vec{U}^{m+1}, \vec{\omega}^m \right\rangle_{\Gamma^m}^h = 0, \tag{5.5b}$$

$$\left\langle \nabla_s \cdot (\vec{\pi}^m \vec{U}^{m+1}), \eta \right\rangle_{\Gamma^m} = 0 \quad \forall \eta \in W(\Gamma^m), \tag{5.5c}$$

$$\left\langle \frac{\vec{X}^{m+1} - \text{id}}{\tau}, \vec{\chi} \right\rangle_{\Gamma^m}^h = \left\langle \vec{U}^{m+1}, \vec{\chi} \right\rangle_{\Gamma^m}^h \quad \forall \vec{\chi} \in \underline{V}(\Gamma^m), \tag{5.5d}$$

$$\langle \vec{\kappa}^{m+1}, \vec{\eta} \rangle_{\Gamma^m}^h + \langle \nabla_s \vec{X}^{m+1}, \nabla_s \vec{\eta} \rangle_{\Gamma^m} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m), \quad (5.6a)$$

$$\langle \underline{\underline{W}}^{m+1}, \underline{\underline{\zeta}} \rangle_{\Gamma^m}^h + \frac{1}{2} \langle \vec{\nu}^m, [\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T] \vec{\kappa}^{m+1} + \nabla_s \cdot [\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T] \rangle_{\Gamma^m}^h = 0 \quad \forall \underline{\underline{\zeta}} \in \underline{\underline{V}}(\Gamma^m), \quad (5.6b)$$

$$\begin{aligned} \langle \vec{Y}^{m+1}, \vec{\xi} \rangle_{\Gamma^m}^h - \langle \alpha^m (\vec{\kappa}^{m+1} - \vec{\varkappa}^m \vec{\nu}^m), \vec{\xi} \rangle_{\Gamma^m}^h \\ - \langle \alpha^{G,m} (\vec{\Pi}_{m-1}^m \vec{\kappa}^m + \underline{\underline{\Pi}}_{m-1}^m \underline{\underline{W}}^m \vec{\nu}^m), \vec{\xi} \rangle_{\Gamma^m}^h = 0 \quad \forall \vec{\xi} \in \underline{V}(\Gamma^m), \end{aligned} \quad (5.6c)$$

$$\begin{aligned} \langle \vec{F}_\Gamma^{m+1}, \vec{\chi} \rangle_{\Gamma^m}^h &= \langle \nabla_s \vec{Y}^{m+1}, \nabla_s \vec{\chi} \rangle_{\Gamma^m} + \langle \nabla_s \cdot (\vec{\Pi}_{m-1}^m \vec{Y}^m), \nabla_s \cdot \vec{\chi} \rangle_{\Gamma^m} \\ &- \frac{1}{2} \langle \alpha^m |\vec{\Pi}_{m-1}^m \vec{\kappa}^m - \vec{\varkappa}^m \vec{\nu}^m|^2 - 2 \vec{\Pi}_{m-1}^m \vec{Y}^m \cdot \vec{\Pi}_{m-1}^m \vec{\kappa}^m, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma^m}^h \\ &- 2 \langle [\nabla_s (\vec{\Pi}_{m-1}^m \vec{Y}^m)]^T, \underline{\underline{D}}_s^m(\vec{\chi}) (\nabla_s \text{id})^T \rangle_{\Gamma^m} - \langle \alpha^m \vec{\varkappa}^m \vec{\Pi}_{m-1}^m \vec{\kappa}^m, [\nabla_s \vec{\chi}]^T \vec{\nu}^m \rangle_{\Gamma^m}^h \\ &- \beta \langle b_{CH}(\mathfrak{C}^m), \nabla_s \cdot \vec{\chi} \rangle_{\Gamma^m}^h + \beta \gamma \langle (\nabla_s \mathfrak{C}^m) \otimes (\nabla_s \mathfrak{C}^m), \nabla_s \vec{\chi} \rangle_{\Gamma^m} \\ &- \frac{1}{2} \langle \alpha^{G,m} (|\vec{\Pi}_{m-1}^m \vec{\kappa}^m|^2 + |\underline{\underline{\Pi}}_{m-1}^m \underline{\underline{W}}^m|^2), \nabla_s \cdot \vec{\chi} \rangle_{\Gamma^m}^h \\ &+ \langle \vec{\nu}^m \cdot (\underline{\underline{Z}}^m \vec{\Pi}_{m-1}^m \vec{\kappa}^m + \nabla_s \cdot \underline{\underline{Z}}^m), \nabla_s \cdot \vec{\chi} \rangle_{\Gamma^m}^h \\ &+ \sum_{i=1}^d \langle \nu_i^m \nabla_s \vec{Z}_i^m, \nabla_s \vec{\chi} - 2 \underline{\underline{D}}_s^m(\vec{\chi}) \rangle_{\Gamma^m} - \langle \underline{\underline{Z}}^m \vec{\kappa}^m + \nabla_s \cdot \underline{\underline{Z}}^m, [\nabla_s \vec{\chi}]^T \vec{\nu}^m \rangle_{\Gamma^m}^h \\ &\quad \forall \vec{\chi} \in \underline{V}(\Gamma^m), \end{aligned} \quad (5.6d)$$

and set $\Gamma^{m+1} = \vec{X}^{m+1}(\Gamma^m)$. Here we have defined $\vec{f}^{m+1} := \vec{I}_2^m \vec{f}(\cdot, t_{m+1})$, $\underline{\underline{Z}}^m = \underline{\underline{\pi}}^m [-\alpha^G(\mathfrak{C}^m) \underline{\underline{\Pi}}_{m-1}^m \underline{\underline{W}}^m]$ and $\vec{Z}_i^m = \underline{\underline{Z}}^m \vec{e}_i$, $i = 1 \rightarrow d$. Having computed Γ^{m+1} , find $\mathfrak{C}^{m+1} \in W_{\leq 1}(\Gamma^{m+1})$ and $\mathfrak{M}^{m+1} \in W(\Gamma^{m+1})$ such that

$$\frac{\vartheta}{\tau} \langle \mathfrak{C}^{m+1}, \chi_k^{m+1} \rangle_{\Gamma^{m+1}}^h + \langle \nabla_s \mathfrak{M}^{m+1}, \nabla_s \chi_k^{m+1} \rangle_{\Gamma^{m+1}} = \frac{\vartheta}{\tau} \langle \mathfrak{C}^m, \chi_k^m \rangle_{\Gamma^m}^h \quad \forall k \in \{1, \dots, K_\Gamma\}. \quad (5.7a)$$

$$\begin{aligned} \beta \gamma \langle \nabla_s \mathfrak{C}^{m+1}, \nabla_s [\chi - \mathfrak{C}^{m+1}] \rangle_{\Gamma^{m+1}} &\geq \langle \mathfrak{M}^{m+1} + \beta \gamma^{-1} \Pi_m^{m+1} \mathfrak{C}^m, \chi - \mathfrak{C}^{m+1} \rangle_{\Gamma^{m+1}}^h \\ &- \frac{1}{2} \langle \alpha'(\Pi_m^{m+1} \mathfrak{C}^m) |\vec{\Pi}_m^{m+1} \vec{\kappa}^{m+1} - \vec{\varkappa}(\Pi_m^{m+1} \mathfrak{C}^m) \vec{\nu}^{m+1}|^2, \chi - \mathfrak{C}^{m+1} \rangle_{\Gamma^{m+1}}^h \\ &+ \langle \vec{\varkappa}'(\Pi_m^{m+1} \mathfrak{C}^m) \alpha(\Pi_m^{m+1} \mathfrak{C}^m) (\vec{\Pi}_m^{m+1} \vec{\kappa}^{m+1} - \vec{\varkappa}(\Pi_m^{m+1} \mathfrak{C}^m) \vec{\nu}^{m+1}) \cdot \vec{\nu}^{m+1}, \chi - \mathfrak{C}^{m+1} \rangle_{\Gamma^{m+1}}^h \\ &- \frac{1}{2} \langle (\alpha^G)'(\Pi_m^{m+1} \mathfrak{C}^m) (|\vec{\Pi}_m^{m+1} \vec{\kappa}^{m+1}|^2 - |\underline{\underline{\Pi}}_m^{m+1} \underline{\underline{W}}^{m+1}|^2), \chi - \mathfrak{C}^{m+1} \rangle_{\Gamma^{m+1}}^h \\ &\quad \forall \chi \in W_{\leq 1}(\Gamma^{m+1}). \end{aligned} \quad (5.7b)$$

Here we note that (5.7a,b) is a fully discrete approximation of (4.17a,b) for the obstacle potential (2.6b).

In the absence of the LBB_Γ condition (5.4) we need to consider the reduced system

(5.5a,d), (5.6a-d), where $\mathbb{U}^m(\vec{0})$ in (5.5a) is replaced by $\mathbb{U}_0^m(\vec{0})$. Here we define

$$\begin{aligned} \mathbb{U}_0^m(\vec{a}) := \left\{ \vec{U} \in \mathbb{U}^m(\vec{a}) : (\nabla \cdot \vec{U}, \varphi) = 0 \quad \forall \varphi \in \widehat{\mathbb{P}}^m, \left\langle \nabla_s \cdot (\vec{\kappa}^m \vec{U}), \eta \right\rangle_{\Gamma^m} = 0 \quad \forall \eta \in W(\Gamma^m) \right. \\ \left. \text{and } \left\langle \vec{U}, \vec{\omega}^m \right\rangle_{\Gamma^m}^h = 0 \right\}, \end{aligned} \quad (5.8)$$

for given data $\vec{a} \in [C(\overline{\Omega})]^d$.

In order to prove the existence of a unique solution to (5.5a-d), (5.6a-d) we make the following very mild well-posedness assumption.

(A) We assume for $m = 0, \dots, M-1$ that $\mathcal{H}^{d-1}(\sigma_j^m) > 0$ for all $j = 1, \dots, J_\Gamma$, and that $\Gamma^m \subset \Omega$.

THEOREM. 5.1. *Let the assumption (A) hold. If the LBB_Γ condition (5.4) holds, then there exists a unique solution $(\vec{U}^{m+1}, P^{m+1}, P_{\text{sing}}^{m+1}, P_\Gamma^{m+1}, \vec{X}^{m+1}, \vec{\kappa}^{m+1}, \vec{Y}^{m+1}, \vec{F}_\Gamma^{m+1}, \underline{W}^{m+1}) \in \mathbb{U}^m(\vec{g}) \times \widehat{\mathbb{P}}^m \times \mathbb{R} \times W(\Gamma^m) \times [\underline{V}(\Gamma^m)]^4 \times \underline{V}(\Gamma^m)$ to (5.5a-d), (5.6a-d). In all other cases, on assuming that $\mathbb{U}_0^m(\vec{g})$ is nonempty, there exists a unique solution $(\vec{U}^{m+1}, \vec{X}^{m+1}, \vec{\kappa}^{m+1}, \vec{Y}^{m+1}, \vec{F}_\Gamma^{m+1}, \underline{W}^{m+1}) \in \mathbb{U}_0^m(\vec{g}) \times [\underline{V}(\Gamma^m)]^4 \times \underline{V}(\Gamma^m)$ to the reduced system (5.5a,d), (5.6a-d) with $\mathbb{U}^m(\vec{0})$ replaced by $\mathbb{U}_0^m(\vec{0})$.*

Proof. As the system (5.5a-d), (5.6a-d) is linear, existence follows from uniqueness. In order to establish the latter, we consider the homogeneous system. Find $(\vec{U}, P, P_{\text{sing}}, P_\Gamma, \vec{X}, \vec{\kappa}, \vec{Y}, \vec{F}_\Gamma, \underline{W}) \in \mathbb{U}^m(\vec{0}) \times \widehat{\mathbb{P}}^m \times \mathbb{R} \times W(\Gamma^m) \times [\underline{V}(\Gamma^m)]^4 \times \underline{V}(\Gamma^m)$ such

that

$$\begin{aligned}
& \frac{1}{2\tau} \left((\rho^m + I_0^m \rho^{m-1}) \vec{U}, \vec{\xi} \right) + 2 \left(\mu^m \underline{\underline{D}}(\vec{U}), \underline{\underline{D}}(\vec{\xi}) \right) - \left(P, \nabla \cdot \vec{\xi} \right) - P_{\text{sing}} \left\langle \vec{\omega}^m, \vec{\xi} \right\rangle_{\Gamma^m}^h \\
& + \frac{1}{2} \left(\rho^m, [(\vec{I}_2^m \vec{U}^m \cdot \nabla) \vec{U}] \cdot \vec{\xi} - [(\vec{I}_2^m \vec{U}^m \cdot \nabla) \vec{\xi}] \cdot \vec{U} \right) \\
& + \frac{1}{\tau} \rho_{\Gamma} \left\langle \vec{U}, \vec{\xi} \right\rangle_{\Gamma^m}^h + 2 \mu_{\Gamma} \left\langle \underline{\underline{D}}_s^m(\vec{\pi}^m \vec{U}), \underline{\underline{D}}_s^m(\vec{\pi}^m \vec{\xi}) \right\rangle_{\Gamma^m} \\
& - \left\langle P_{\Gamma}, \nabla_s \cdot (\vec{\pi}^m \vec{\xi}) \right\rangle_{\Gamma^m} - \left\langle \vec{F}_{\Gamma}, \vec{\xi} \right\rangle_{\Gamma^m}^h = 0 \quad \forall \vec{\xi} \in \mathbb{U}^m(\vec{0}), \tag{5.9a}
\end{aligned}$$

$$\left(\nabla \cdot \vec{U}, \varphi \right) = 0 \quad \forall \varphi \in \widehat{\mathbb{P}}^m \quad \text{and} \quad \left\langle \vec{U}, \vec{\omega}^m \right\rangle_{\Gamma^m}^h = 0, \tag{5.9b}$$

$$\left\langle \nabla_s \cdot (\vec{\pi}^m \vec{U}), \eta \right\rangle_{\Gamma^m} = 0 \quad \forall \eta \in W(\Gamma^m), \tag{5.9c}$$

$$\frac{1}{\tau} \left\langle \vec{X}, \vec{\chi} \right\rangle_{\Gamma^m}^h = \left\langle \vec{U}, \vec{\chi} \right\rangle_{\Gamma^m}^h \quad \forall \vec{\chi} \in \underline{V}(\Gamma^m), \tag{5.9d}$$

$$\left\langle \vec{\kappa}, \vec{\eta} \right\rangle_{\Gamma^m}^h + \left\langle \nabla_s \vec{X}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^m} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m), \tag{5.9e}$$

$$\left\langle \underline{\underline{W}}, \underline{\underline{\zeta}} \right\rangle_{\Gamma^m}^h + \frac{1}{2} \left\langle \vec{\nu}^m, [\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T] \vec{\kappa} \right\rangle_{\Gamma^m}^h = 0 \quad \forall \underline{\underline{\zeta}} \in \underline{\underline{V}}(\Gamma^m), \tag{5.9f}$$

$$\left\langle \vec{Y}, \vec{\eta} \right\rangle_{\Gamma^m}^h - \left\langle \alpha^m \vec{\kappa}, \vec{\eta} \right\rangle_{\Gamma^m}^h = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^m), \tag{5.9g}$$

$$\left\langle \vec{F}_{\Gamma}, \vec{\chi} \right\rangle_{\Gamma^m}^h - \left\langle \nabla_s \vec{Y}, \nabla_s \vec{\chi} \right\rangle_{\Gamma^m} = 0 \quad \forall \vec{\chi} \in \underline{V}(\Gamma^m). \tag{5.9h}$$

Choosing $\vec{\xi} = \vec{U}$ in (5.9a), $\varphi = P$ in (5.9b), $\eta = P_{\Gamma}$ in (5.9c), $\vec{\chi} = \vec{F}_{\Gamma}$ in (5.9d), $\vec{\chi} = \vec{X}$ in (5.9h), $\vec{\eta} = \vec{Y}$ in (5.9e) and $\vec{\eta} = \vec{\kappa}$ in (5.9g) yields that

$$\begin{aligned}
& \frac{1}{2} \left((\rho^m + I_0^m \rho^{m-1}) \vec{U}, \vec{U} \right) + 2\tau \left(\mu^m \underline{\underline{D}}(\vec{U}), \underline{\underline{D}}(\vec{U}) \right) + \rho_{\Gamma} \left\langle \vec{U}, \vec{U} \right\rangle_{\Gamma^m}^h \\
& + 2\tau \mu_{\Gamma} \left\langle \underline{\underline{D}}_s^m(\vec{\pi}^m \vec{U}), \underline{\underline{D}}_s^m(\vec{\pi}^m \vec{U}) \right\rangle_{\Gamma^m} \\
& = \tau \left\langle \vec{F}_{\Gamma}, \vec{U} \right\rangle_{\Gamma^m}^h = \left\langle \vec{F}_{\Gamma}, \vec{X} \right\rangle_{\Gamma^m}^h = \left\langle \nabla_s \vec{Y}, \nabla_s \vec{X} \right\rangle_{\Gamma^m} = - \left\langle \vec{\kappa}, \vec{Y} \right\rangle_{\Gamma^m}^h \\
& = - \left\langle \alpha^m \vec{\kappa}, \vec{\kappa} \right\rangle_{\Gamma^m}^h. \tag{5.10}
\end{aligned}$$

It immediately follows from (5.10), Korn's inequality and $\alpha^m > 0$, that $\vec{U} = \vec{0} \in \mathbb{U}^m(\vec{0})$ and $\vec{\kappa} = \vec{0}$. (For the application of Korn's inequality we recall that $\mathcal{H}^{d-1}(\partial_1 \Omega) > 0$.) Hence (5.9d,f,g,h) yield that $\vec{X} = \vec{0}$, $\underline{\underline{W}} = \underline{\underline{0}}$, $\vec{Y} = \vec{0}$ and $\vec{F}_{\Gamma} = \vec{0}$, respectively. Finally, if (5.4) holds then (5.9a) with $\vec{U} = \vec{0}$ and $\vec{F}_{\Gamma} = \vec{0}$ implies that $P = 0 \in \widehat{\mathbb{P}}^m$, $P_{\text{sing}} = 0$ and $P_{\Gamma} = 0 \in W(\Gamma^m)$. This shows existence and uniqueness of $(\vec{U}^{m+1}, P^{m+1}, P_{\text{sing}}^{m+1}, P_{\Gamma}^{m+1}, \vec{X}^{m+1}, \vec{\kappa}^{m+1}, \vec{Y}^{m+1}, \vec{F}_{\Gamma}^{m+1}, \underline{\underline{W}}^{m+1}) \in \mathbb{U}^m(\vec{g}) \times \widehat{\mathbb{P}}^m \times \mathbb{R} \times W(\Gamma^m) \times [\underline{V}(\Gamma^m)]^4 \times \underline{\underline{V}}(\Gamma^m)$ to (5.5a-d), (5.6a-d). The proof for the reduced system is very similar. The homogeneous system to consider is (5.9a,d-h) with $\mathbb{U}^m(\vec{0})$ replaced by $\mathbb{U}_0^m(\vec{0})$. As before, we infer that (5.10) holds, which yields that $\vec{U} = \vec{0} \in \mathbb{U}_0^m(\vec{0})$, $\vec{\kappa} = \vec{0}$, and hence $\vec{X} = \vec{F}_{\Gamma} = \vec{Y} = \vec{0}$.

In order to prove the existence of a unique solution to (5.7a,b), we adapt the argument in Blowey and Elliott (1992) for the Cahn–Hilliard equation with obstacle potential on

a bounded fixed domain in \mathbb{R}^d . We introduce the discrete inverse surface Laplacian $\mathcal{G}^{m+1} : W_f(\Gamma^{m+1}) \rightarrow W_f(\Gamma^{m+1})$ defined by

$$\langle \nabla_s \mathcal{G}^{m+1} v, \nabla_s \xi \rangle_{\Gamma^{m+1}} = \langle v, \xi \rangle_{\Gamma^{m+1}}^h \quad \forall \xi \in W_f(\Gamma^{m+1}), \quad (5.11)$$

where $W_f(\Gamma^{m+1}) := \{\xi \in W(\Gamma^{m+1}) : \langle \xi, 1 \rangle_{\Gamma^{m+1}} = 0\}$. It immediately follows from $\langle \nabla_s v, \nabla_s v \rangle_{\Gamma^{m+1}} = 0 \Rightarrow v = 0$ for all $v \in W_f(\Gamma^{m+1})$ that \mathcal{G}^{m+1} is well-posed. Next we rewrite (5.7a,b) as

$$\frac{\vartheta}{\tau} \left\langle \mathfrak{C}^{m+1} - \widehat{\mathfrak{C}}^m, \chi_k^{m+1} \right\rangle_{\Gamma^{m+1}}^h + \langle \nabla_s \mathfrak{M}^{m+1}, \nabla_s \chi_k^{m+1} \rangle_{\Gamma^{m+1}} = 0 \quad \forall k \in \{1, \dots, K_\Gamma\}. \quad (5.12a)$$

$$\beta \gamma \langle \nabla_s \mathfrak{C}^{m+1}, \nabla_s [\chi - \mathfrak{C}^{m+1}] \rangle_{\Gamma^{m+1}} \geq \langle \mathfrak{M}^{m+1} + g, \chi - \mathfrak{C}^{m+1} \rangle_{\Gamma^{m+1}}^h \quad \forall \chi \in W_{\leq 1}(\Gamma^{m+1}), \quad (5.12b)$$

where $\widehat{\mathfrak{C}}^m \in W(\Gamma^{m+1})$ is such that $\langle \widehat{\mathfrak{C}}^m, \chi_k^{m+1} \rangle_{\Gamma^{m+1}}^h = \langle \mathfrak{C}^m, \chi_k^m \rangle_{\Gamma^m}^h$ for $k \in \{1, \dots, K_\Gamma\}$. We note that

$$\langle \mathfrak{C}^{m+1}, 1 \rangle_{\Gamma^{m+1}} = \langle \widehat{\mathfrak{C}}^m, 1 \rangle_{\Gamma^{m+1}} = \langle \mathfrak{C}^m, 1 \rangle_{\Gamma^m}. \quad (5.13)$$

It follows from (5.13), (5.12a) and (5.11) that

$$\mathfrak{M}^{m+1} = -\frac{\vartheta}{\tau} \mathcal{G}^{m+1} (\mathfrak{C}^{m+1} - \widehat{\mathfrak{C}}^m) + \lambda^{m+1}, \quad (5.14)$$

where $\lambda^{m+1} \in \mathbb{R}$ is a Lagrange multiplier associated with the constraint (5.13). Hence $\mathfrak{C}^{m+1} \in W_{\leq 1}(\Gamma^{m+1})$ is such that $\langle \mathfrak{C}^{m+1}, 1 \rangle_{\Gamma^{m+1}} = \langle \mathfrak{C}^m, 1 \rangle_{\Gamma^m}$ and

$$\begin{aligned} \beta \gamma \langle \nabla_s \mathfrak{C}^{m+1}, \nabla_s [\chi - \mathfrak{C}^{m+1}] \rangle_{\Gamma^{m+1}} + \frac{\vartheta}{\tau} \left\langle \mathcal{G}^{m+1} (\mathfrak{C}^{m+1} - \widehat{\mathfrak{C}}^m) - \lambda^{m+1} - g, \chi - \mathfrak{C}^{m+1} \right\rangle_{\Gamma^{m+1}}^h \\ \geq 0 \quad \forall \chi \in W_{\leq 1}(\Gamma^{m+1}). \end{aligned} \quad (5.15)$$

Clearly, (5.15) is the Euler–Lagrange variational inequality for the strictly convex minimization problem

$$\begin{aligned} \min_{\substack{\chi \in W_{\leq 1}(\Gamma^{m+1}) \\ \langle \chi, 1 \rangle_{\Gamma^{m+1}} = \langle \mathfrak{C}^m, 1 \rangle_{\Gamma^m}}} \left[\frac{\beta \gamma}{2} \langle \nabla_s \chi, \nabla_s \chi \rangle_{\Gamma^{m+1}} + \frac{\vartheta}{2\tau} \left\langle \nabla_s \mathcal{G}^{m+1} (\chi - \widehat{\mathfrak{C}}^m), \nabla_s \mathcal{G}^{m+1} (\chi - \widehat{\mathfrak{C}}^m) \right\rangle_{\Gamma^{m+1}}^h \right. \\ \left. - \frac{\vartheta}{\tau} \langle g, \chi \rangle_{\Gamma^{m+1}}^h \right]. \end{aligned} \quad (5.16)$$

Hence there exists a unique $\mathfrak{C}^{m+1} \in W_{\leq 1}(\Gamma^{m+1})$ with $\langle \mathfrak{C}^{m+1}, 1 \rangle_{\Gamma^{m+1}} = \langle \mathfrak{C}^m, 1 \rangle_{\Gamma^m}$ and solving (5.15). Existence of the Lagrange multiplier λ^{m+1} in (5.14) then follows from a fixed point argument, see Blowey and Elliott (1992, p. 151). \square

6 Solution methods

In this section we briefly describe possible solution methods for the linear system (5.5a–d), (5.6a–d), where we note that (5.6b) decouples from the remaining equations, and for the nonlinear system (5.7a,b).

In order to derive the linear system of equations for the coefficient vectors of the finite element functions $(\vec{U}^{m+1}, P^{m+1}, P_{\text{sing}}^{m+1}, P_{\Gamma}^{m+1}, \delta \vec{X}^{m+1}, \vec{\kappa}^{m+1}, \vec{Y}^{m+1}, \vec{F}_{\Gamma}^{m+1})$ corresponding to (5.5a–d), (5.6a,c,d), where $\delta \vec{X}^{m+1} = \vec{X}^{m+1} - \text{id}|_{\Gamma^m}$, we begin by introducing the following matrices and vectors, where we closely follow our previous work in Barrett et al. (2016a). Let $i, j = 1, \dots, K_{\mathbb{U}}^m$, $n, q = 1, \dots, K_{\mathbb{P}}^m$ and $k, l = 1, \dots, K_{\Gamma}$. Then

$$\begin{aligned}
[\vec{B}_{\Omega}]_{ij} &:= \left(\frac{\rho^m + I_0^m \rho^{m-1}}{2\tau} \phi_j^{\mathbb{U}^m}, \phi_i^{\mathbb{U}^m} \right) \underline{\text{Id}} + 2 \left((\mu^m \underline{D}(\phi_j^{\mathbb{U}^m} \vec{e}_r), \underline{D}(\phi_i^{\mathbb{U}^m} \vec{e}_s)) \right)_{r,s=1}^d \\
&\quad + \frac{1}{2} \left(\rho^m, [(\vec{I}_2^m \vec{U}^m \cdot \nabla) \phi_j^{\mathbb{U}^m}] \phi_i^{\mathbb{U}^m} - [(\vec{I}_2^m \vec{U}^m \cdot \nabla) \phi_i^{\mathbb{U}^m}] \phi_j^{\mathbb{U}^m} \right) \underline{\text{Id}}, \\
&\quad + \frac{\rho_{\Gamma}}{\tau} \langle \phi_j^{\mathbb{U}^m}, \phi_i^{\mathbb{U}^m} \rangle_{\Gamma^m}^h \underline{\text{Id}} + 2\mu_{\Gamma} \left(\langle \underline{D}_s^m(\pi^m \phi_j^{\mathbb{U}^m} \vec{e}_r), \underline{D}_s^m(\pi^m \phi_i^{\mathbb{U}^m} \vec{e}_s) \rangle_{\Gamma^m} \right)_{r,s=1}^d \\
[\vec{C}_{\Omega}]_{iq} &:= -(\phi_q^{\mathbb{P}^m}, (\nabla \cdot (\phi_i^{\mathbb{U}^m} \vec{e}_r)))_{r=1}^d, \quad [\vec{S}_{\Gamma, \Omega}]_{il} := -(\langle \chi_l^m, \nabla_s \cdot (\pi^m \phi_i^{\mathbb{U}^m} \vec{e}_r) \rangle_{\Gamma^m})_{r=1}^d, \\
\vec{b}_i &= \left(\frac{I_0^m \rho^{m-1}}{\tau} \vec{I}_2^m \vec{U}^m + \rho^m \vec{f}^{m+1}, \phi_i^{\mathbb{U}^m} \right) + \frac{\rho_{\Gamma}}{\tau} \left\langle \vec{\Pi}_{m-1}^m \vec{U}^m|_{\Gamma^{m-1}}, \phi_i^{\mathbb{U}^m} \right\rangle_{\Gamma^m}^h \\
&\quad - \frac{1}{2} \rho_+ \left\langle (\vec{U}^m \cdot \vec{n}) \vec{U}^m, \phi_i^{\mathbb{U}^m} \right\rangle_{\partial_2 \Omega}; \tag{6.1}
\end{aligned}$$

where $\{\vec{e}_r\}_{r=1}^d$ denotes the standard basis in \mathbb{R}^d , and where we have used the convention that the subscripts in the matrix notations refer to the test and trial domains, respectively. A single subscript is used where the two domains are the same. The entries of \vec{D}_{Ω} , for $i = 1, \dots, K_{\mathbb{U}}^m$, are given by $[\vec{D}_{\Omega}]_{i,1} := -\langle \phi_i^{\mathbb{U}^m}, \vec{\omega}^m \rangle_{\Gamma^m}^h$.

In order to provide a matrix-vector formulation for the full system (5.5a–d), (5.6a,c,d), and in particular in view of (5.6c), we recall from Dziuk (2008, p. 64) that

$$\begin{aligned}
&2 \left\langle (\nabla_s \vec{\xi})^T, \underline{D}_s^m(\vec{\chi}) (\nabla_s \text{id})^T \right\rangle_{\Gamma^m} \\
&= \sum_{i,j=1}^d \left\langle (\nabla_s)_j (\vec{\xi})_i, (\nabla_s)_i (\vec{\chi})_j \right\rangle_{\Gamma^m} - \sum_{i,j=1}^d \left\langle (\vec{\nu}^m)_i (\vec{\nu}^m)_j \nabla_s (\vec{\xi})_j, \nabla_s (\vec{\chi})_i \right\rangle_{\Gamma^m} \\
&\quad + \left\langle \nabla_s \vec{\xi}, \nabla_s \vec{\chi} \right\rangle_{\Gamma^m} \\
&= \sum_{i,j=1}^d \left\langle (\nabla_s)_j (\vec{\xi})_i, (\nabla_s)_i (\vec{\chi})_j \right\rangle_{\Gamma^m} + \sum_{i,j=1}^d \left\langle (\delta_{ij} - (\vec{\nu}^m)_i (\vec{\nu}^m)_j) \nabla_s (\vec{\xi})_j, \nabla_s (\vec{\chi})_i \right\rangle_{\Gamma^m}.
\end{aligned}$$

Moreover, we observe that $\langle \nabla_s \cdot \vec{\xi}, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma^m} = \sum_{i,j=1}^d \langle (\nabla_s)_j (\vec{\xi})_j, (\nabla_s)_i (\vec{\chi})_i \rangle_{\Gamma^m}$. Hence, in addition to (6.1), we introduce the following matrices and vectors, where $q = 1, \dots, K_{\mathbb{U}}^m$,

and $k, l = 1, \dots, K_\Gamma$

$$\begin{aligned}
[\vec{\mathcal{B}}_\Gamma]_{kl} &:= (\langle [\nabla_s]_j \chi_l^m, [\nabla_s]_i \chi_k^m \rangle_{\Gamma^m})_{i,j=1}^d, & [\vec{\mathcal{R}}_\Gamma]_{kl} &:= \langle \nabla_s \chi_l^m \cdot \nabla_s \chi_k^m, \underline{\text{Id}} - \vec{\nu}^m \otimes \vec{\nu}^m \rangle_{\Gamma^m}, \\
[\vec{M}_{\Gamma,\Omega}]_{ql} &:= \langle \chi_l^m, \phi_q^{\mathbb{U}^m} \rangle_{\Gamma^m} \underline{\text{Id}}, & [\vec{M}_\Gamma]_{kl} &:= \langle \chi_l^m, \chi_k^m \rangle_{\Gamma^m}^h \underline{\text{Id}}, \\
[\vec{M}_{\Gamma,\alpha}]_{kl} &:= \langle \alpha^m \chi_l^m, \chi_k^m \rangle_{\Gamma^m}^h \underline{\text{Id}}, & [A_\Gamma]_{kl} &:= \langle \nabla_s \chi_l^m, \nabla_s \chi_k^m \rangle_{\Gamma^m}, & [\vec{A}_\Gamma]_{kl} &:= [A_\Gamma]_{kl} \underline{\text{Id}}, \\
\vec{c}_k &:= -\langle \alpha^m \vec{\mathcal{Z}}^m \vec{\nu}^m, \chi_k^m \rangle_{\Gamma^m}^h + \left\langle \alpha^{G,m} (\vec{\Pi}_{m-1}^m \vec{\kappa}^m + \underline{\Pi}_{m-1}^m \underline{W}^m \vec{\nu}^m), \chi_k^m \right\rangle_{\Gamma^m}^h, \\
[\vec{d}_\alpha]_k &:= \left\langle \alpha^m \vec{\mathcal{Z}}^m, (\vec{\Pi}_{m-1}^m \vec{\kappa}^m \cdot \nabla_s \chi_k^m) \vec{\nu}^m \right\rangle_{\Gamma^m}^h, \\
[\vec{d}_\kappa]_k &:= \frac{1}{2} \left\langle \alpha^m |\vec{\Pi}_{m-1}^m \vec{\kappa}^m - \vec{\mathcal{Z}}^m \vec{\nu}^m|^2 - 2 \vec{\Pi}_{m-1}^m \vec{Y}^m \cdot \vec{\Pi}_{m-1}^m \vec{\kappa}^m, \nabla_s \chi_k^m \right\rangle_{\Gamma^m}^h, \\
[\vec{d}_\beta]_k &:= \beta \langle b_{CH}(\mathfrak{E}^m), \nabla_s \chi_k^m \rangle_{\Gamma^m}^h - \beta \gamma (\langle (\nabla_s \mathfrak{E}^m) \otimes (\nabla_s \mathfrak{E}^m), \vec{e}_r \otimes \nabla_s \chi_k^m \rangle_{\Gamma^m})_{r=1}^d \\
&= \beta \langle b_{CH}(\mathfrak{E}^m), \nabla_s \chi_k^m \rangle_{\Gamma^m}^h - \beta \gamma \langle \nabla_s \mathfrak{E}^m \cdot \nabla_s \chi_k^m, \nabla_s \mathfrak{E}^m \rangle_{\Gamma^m}, \\
[\vec{d}_G]_k &:= \frac{1}{2} \left\langle \alpha^{G,m} (|\vec{\Pi}_{m-1}^m \vec{\kappa}^m|^2 + |\underline{\Pi}_{m-1}^m \underline{W}^m|^2), \nabla_s \chi_k^m \right\rangle_{\Gamma^m}^h, \\
[\vec{d}_Z]_k &:= \left\langle (\underline{Z}^m \vec{\Pi}_{m-1}^m \vec{\kappa}^m + \nabla_s \cdot \underline{Z}^m) \cdot \nabla_s \chi_k^m, \vec{\nu}^m \right\rangle_{\Gamma^m}^h - \left\langle (\underline{Z}^m \vec{\Pi}_{m-1}^m \vec{\kappa}^m + \nabla_s \cdot \underline{Z}^m) \cdot \vec{\nu}^m, \nabla_s \chi_k^m \right\rangle_{\Gamma^m}^h \\
&\quad - \sum_{i=1}^d \left(\left\langle \nu_i^m \nabla_s \vec{Z}_i^m, \nu_r^m [\vec{\nu}^m \otimes \nabla_s \chi_k^m] - \nabla_s \chi_k^m \otimes \vec{e}_r \right\rangle_{\Gamma^m} \right)_{r=1}^d.
\end{aligned}$$

Here we have made use of the facts that

$$\begin{aligned}
[\vec{\mathcal{B}}_\Gamma]_{kl} &= (\langle \nabla_s \cdot (\chi_l^m \vec{e}_j), \nabla_s \cdot (\chi_k^m \vec{e}_i) \rangle_{\Gamma^m})_{i,j=1}^d = (\langle (\nabla_s \chi_l^m) \cdot \vec{e}_j, (\nabla_s \chi_k^m) \cdot \vec{e}_i \rangle_{\Gamma^m})_{i,j=1}^d \\
&= (\langle [\nabla_s]_j \chi_l^m, [\nabla_s]_i \chi_k^m \rangle_{\Gamma^m})_{i,j=1}^d
\end{aligned}$$

and that

$$\begin{aligned}
&\left(\left\langle \nu_i^m \nabla_s \vec{Z}_i^m, \vec{e}_r \otimes \nabla_s \chi_k^m - \underline{\mathcal{P}}_{\Gamma^m} [\vec{e}_r \otimes \nabla_s \chi_k^m] - [\nabla_s \chi_k^m \otimes \vec{e}_r] \underline{\mathcal{P}}_{\Gamma^m} \right\rangle_{\Gamma^m} \right)_{r=1}^d \\
&= \left(\left\langle \nu_i^m \nabla_s \vec{Z}_i^m, [\vec{\nu}^m \otimes \vec{\nu}^m] [\vec{e}_r \otimes \nabla_s \chi_k^m] - \nabla_s \chi_k^m \otimes \vec{e}_r + [\nabla_s \chi_k^m \otimes \vec{e}_r] [\vec{\nu}^m \otimes \vec{\nu}^m] \right\rangle_{\Gamma^m} \right)_{r=1}^d \\
&= \left(\left\langle \nu_i^m \nabla_s \vec{Z}_i^m, \nu_r^m [\vec{\nu}^m \otimes \nabla_s \chi_k^m] - \nabla_s \chi_k^m \otimes \vec{e}_r + \nu_r^m [\nabla_s \chi_k^m \otimes \vec{\nu}^m] \right\rangle_{\Gamma^m} \right)_{r=1}^d \\
&= \left(\left\langle \nu_i^m \nabla_s \vec{Z}_i^m, \nu_r^m [\vec{\nu}^m \otimes \nabla_s \chi_k^m] - \nabla_s \chi_k^m \otimes \vec{e}_r \right\rangle_{\Gamma^m} \right)_{r=1}^d
\end{aligned}$$

for $i = 1, \dots, d$, on noting that $\nabla_s \vec{Z}_i^m : [\nabla_s \chi_k^m \otimes \vec{\nu}^m] = [(\nabla_s \vec{Z}_i^m) \vec{\nu}^m] \cdot \nabla_s \chi_k^m = \vec{0} \cdot \nabla_s \chi_k^m = 0$. Moreover, it clearly holds that $([\vec{\mathcal{B}}_\Gamma]_{kl})^T = [\vec{\mathcal{B}}_\Gamma]_{lk} =: [\vec{\mathcal{B}}_\Gamma^*]_{kl}$.

Denoting the system matrix

$$\begin{pmatrix} \vec{B}_\Omega & \vec{C}_\Omega & \vec{D}_\Omega & \vec{S}_{\Gamma,\Omega} \\ \vec{C}_\Omega^T & 0 & 0 & 0 \\ \vec{D}_\Omega^T & 0 & 0 & 0 \\ \vec{S}_{\Gamma,\Omega}^T & 0 & 0 & 0 \end{pmatrix}$$

as $\begin{pmatrix} \vec{B}_\Omega & \vec{c} \\ \vec{c}^T & 0 \end{pmatrix}$, and letting $\tilde{P}^{m+1} = (P^{m+1}, P_{\text{sing}}^{m+1}, P_\Gamma^{m+1})^T$, then the linear system (5.5a–d), (5.6a,c,d) can be written as

$$\begin{pmatrix} \vec{B}_\Omega & \vec{c} & 0 & 0 & 0 & -\vec{M}_{\Gamma,\Omega} \\ \vec{c}^T & 0 & 0 & 0 & 0 & 0 \\ (\vec{M}_{\Gamma,\Omega})^T & 0 & 0 & -\frac{1}{\tau}\vec{M}_\Gamma & 0 & 0 \\ 0 & 0 & \vec{M}_\Gamma & \vec{A}_\Gamma & 0 & 0 \\ 0 & 0 & -\vec{M}_{\Gamma,\alpha} & 0 & \vec{M}_\Gamma & 0 \\ 0 & 0 & 0 & 0 & -\vec{A}_\Gamma & \vec{M}_\Gamma \end{pmatrix} \begin{pmatrix} \vec{U}^{m+1} \\ \tilde{P}^{m+1} \\ \vec{\kappa}^{m+1} \\ \delta\vec{X}^{m+1} \\ \vec{Y}^{m+1} \\ \vec{F}_\Gamma^{m+1} \end{pmatrix} = \begin{pmatrix} \vec{b} \\ 0 \\ 0 \\ -\vec{A}_\Gamma \vec{X}^m \\ \vec{c} \\ \vec{Z}_\Gamma \vec{Y}^m - \vec{d} \end{pmatrix}, \quad (6.2)$$

where $\vec{Z}_\Gamma := \vec{B}_\Gamma - \vec{B}_\Gamma^* - \vec{R}_\Gamma$ and $\vec{d} = \vec{d}_\kappa + \vec{d}_\alpha + \vec{d}_\beta + \vec{d}_G$. For the solution of (6.2) a Schur complement approach similar to Barrett et al. (2016a) can be used. In particular, the Schur approach for eliminating $(\vec{\kappa}^{m+1}, \delta\vec{X}^{m+1}, \vec{Y}^{m+1}, \vec{F}_\Gamma^{m+1})$ from (6.2) can be obtained as follows. Let

$$\Theta_\Gamma := \begin{pmatrix} 0 & -\frac{1}{\tau}\vec{M}_\Gamma & 0 & 0 \\ \vec{M}_\Gamma & \vec{A}_\Gamma & 0 & 0 \\ -\vec{M}_{\Gamma,\alpha} & 0 & \vec{M}_\Gamma & 0 \\ 0 & 0 & -\vec{A}_\Gamma & \vec{M}_\Gamma \end{pmatrix}.$$

Then (6.2) can be reduced to

$$\begin{pmatrix} \vec{B}_\Omega + \alpha \vec{T}_\Omega & \vec{c} \\ \vec{c}^T & 0 \end{pmatrix} \begin{pmatrix} \vec{U}^{m+1} \\ \tilde{P}^{m+1} \end{pmatrix} = \begin{pmatrix} \vec{b} + \alpha \vec{g} \\ 0 \end{pmatrix} \quad (6.3a)$$

and

$$\begin{pmatrix} \vec{\kappa}^{m+1} \\ \delta\vec{X}^{m+1} \\ \vec{Y}^{m+1} \\ \vec{F}_\Gamma^{m+1} \end{pmatrix} = \Theta_\Gamma^{-1} \begin{pmatrix} -(\vec{M}_{\Gamma,\Omega})^T \vec{U}^{m+1} \\ -\vec{A}_\Gamma \vec{X}^m \\ \vec{c} \\ \vec{Z}_\Gamma \vec{Y}^m - \vec{d} \end{pmatrix}. \quad (6.3b)$$

In (6.3a) we have used the definitions

$$\vec{T}_\Omega = (0 \ 0 \ 0 \ \vec{M}_{\Gamma,\Omega}) \Theta_\Gamma^{-1} \begin{pmatrix} (\vec{M}_{\Gamma,\Omega})^T \\ 0 \\ 0 \\ 0 \end{pmatrix} = \tau \vec{M}_{\Gamma,\Omega} \vec{M}_\Gamma^{-1} \vec{A}_\Gamma \vec{M}_\Gamma^{-1} \vec{M}_{\Gamma,\alpha} \vec{M}_\Gamma^{-1} \vec{A}_\Gamma \vec{M}_\Gamma^{-1} (\vec{M}_{\Gamma,\Omega})^T$$

and

$$\vec{g} = (0 \ 0 \ 0 \ \vec{M}_{\Gamma,\Omega}) \Theta_\Gamma^{-1} \begin{pmatrix} 0 \\ -\vec{A}_\Gamma \vec{X}^m \\ \vec{c} \\ \vec{Z}_\Gamma \vec{Y}^m - \vec{d} \end{pmatrix}.$$

For the linear system (6.3a) well-known solution methods for finite element discretizations for the standard Navier–Stokes equations may be employed. We refer to Barrett et al. (2015, §5), where we describe such solution methods in detail for a very similar situation.

The nonlinear system of algebraic equations arising from the discrete surface Cahn–Hilliard equation (5.7a,b) can be solved in the same way that such variational inequalities for standard Cahn–Hilliard equations are solved. In practice we employ the projection Gauss–Seidel method from Barrett et al. (2004), or the Uzawa-type iteration from Barrett et al. (2014).

7 Numerical results

We implemented the scheme (5.5a–d), (5.6a–d), (5.7a,b) with the help of the finite element toolbox ALBERTA, see Schmidt and Siebert (2005). For the bulk mesh adaptation in our numerical computations we use the strategy from Barrett et al. (2015), which results in a fine mesh around Γ^m and a coarse mesh further away from it.

Given the initial triangulation Γ^0 and $\mathfrak{C}^0 \in W(\Gamma^0)$, with $\mathfrak{C}^0 \in [-1, 1]$, the initial data $\vec{Y}^0 \in \underline{V}(\Gamma^0)$, $\vec{\kappa}^0 \in \underline{V}(\Gamma^0)$ and $\underline{\underline{W}}^0 \in \underline{\underline{V}}(\Gamma^0)$ are always computed as

$$\left\langle \vec{Y}^0, \vec{\eta} \right\rangle_{\Gamma^0}^h = \left\langle \alpha(\mathfrak{C}^0) (\vec{\kappa}^0 - \overline{\mathfrak{K}}(\mathfrak{C}^0) \vec{\nu}^0) - \alpha^G(\mathfrak{C}^0) (\vec{\kappa}^0 + \underline{\underline{W}}^0 \vec{\nu}^0), \vec{\eta} \right\rangle_{\Gamma^0}^h \quad \forall \vec{\eta} \in \underline{V}(\Gamma^0),$$

where $\vec{\kappa}^0 \in \underline{V}(\Gamma^0)$ is the solution to

$$\left\langle \vec{\kappa}^0, \vec{\eta} \right\rangle_{\Gamma^0}^h + \left\langle \nabla_s \text{id}, \nabla_s \vec{\eta} \right\rangle_{\Gamma^0} = 0 \quad \forall \vec{\eta} \in \underline{V}(\Gamma^0),$$

and where $\underline{\underline{W}}^0 \in \underline{\underline{V}}(\Gamma^0)$ is the solution to

$$\left\langle \underline{\underline{W}}^0, \underline{\underline{\zeta}} \right\rangle_{\Gamma^0}^h + \frac{1}{2} \left\langle \vec{\nu}^0, [\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T] \vec{\kappa}^0 + \nabla_s \cdot [\underline{\underline{\zeta}} + \underline{\underline{\zeta}}^T] \right\rangle_{\Gamma^0}^h = 0 \quad \forall \underline{\underline{\zeta}} \in \underline{\underline{V}}(\Gamma^0).$$

Throughout this section we set

$$\alpha(s) = \alpha_L(s) := \frac{1}{2} (\alpha_+ + \alpha_-) + \frac{1}{2} (\alpha_+ - \alpha_-) s, \quad (7.1a)$$

$$\overline{\mathfrak{K}}(s) = \frac{1}{2} (\overline{\mathfrak{K}}_+ + \overline{\mathfrak{K}}_-) + \frac{1}{2} (\overline{\mathfrak{K}}_+ - \overline{\mathfrak{K}}_-) s, \quad (7.1b)$$

$$\alpha^G(s) = \frac{1}{2} (\alpha_+^G + \alpha_-^G) + \frac{1}{2} (\alpha_+^G - \alpha_-^G) s. \quad (7.1c)$$

We recall from the discussion around (1.3) that it follows from (7.1c), (1.2a) and (1.3) that only the difference $(\alpha_+^G - \alpha_-^G)$ plays a role in the evolutions with Gaussian curvature. Moreover, for the choices (7.1a,c) the constraint (1.4) reduces to

$$\min\{\alpha_-, \alpha_+\} \geq \frac{1}{2} |\alpha_+^G - \alpha_-^G|. \quad (7.2)$$

Unless otherwise stated, we use $\rho_{\pm} = 0$, $\mu_{\pm} = 1$, $\mu_{\Gamma} = 1$, $\rho_{\Gamma} = 0$, $\alpha_{\pm} = 1$, $\overline{\mathfrak{K}}_{\pm} = 0$ and $\alpha_{\pm}^G = 0$. Moreover, we normally use $\vartheta = \beta = 1$.

At times we will discuss the discrete energy of the numerical solutions. On recalling Theorem 4.2 and (5.3), the discrete energy is defined by

$$\mathcal{E}_{total}^h = \mathcal{E}_{kin}^h + \mathcal{E}_{\kappa}^h + \mathcal{E}_{CH}^h,$$

where

$$\begin{aligned}\mathcal{E}_{kin}^h &= \frac{1}{2} \|[\rho^m]^{\frac{1}{2}} \vec{U}^{m+1}\|_0^2 + \frac{1}{2} \rho_\Gamma \left\langle \vec{U}^{m+1}, \vec{U}^{m+1} \right\rangle_{\Gamma^m}^h, \\ \mathcal{E}_\kappa^h &= \frac{1}{2} \left\langle \alpha^m, |\vec{\kappa}^{m+1} - \vec{\kappa}^m|^2 \right\rangle_{\Gamma^m}^h + \frac{1}{2} \left\langle \alpha^{G,m}, |\vec{\kappa}^{m+1}|^2 - |\underline{W}^{m+1}|^2 \right\rangle_{\Gamma^m}^h, \\ \mathcal{E}_{CH}^h &= \beta \left\langle b_{CH}(\mathfrak{C}^m), 1 \right\rangle_{\Gamma^m}^h,\end{aligned}$$

represent the kinetic, curvature and Cahn–Hilliard parts of the discrete energy.

In plots where we show the concentration \mathfrak{C}^m in grey scales, the colour scales linearly with \mathfrak{C}^m ranging from -1 (white) to 1 (black).

7.1 Numerical simulations in 2d

We start with an initial shape in the form of a smooth letter “C”. The curve has length 2.823 and we use 257 elements on it. For our choice of $\gamma = 0.02$ this yields on average about 6 elements across the interface, which asymptotically has thickness $\gamma\pi$. The time step size is $\tau = 5 \times 10^{-4}$. For the computational domain we choose $\Omega = (-1, 1)^2$, and we choose a random distribution for \mathfrak{C}^0 with mean value -0.4 . An experiment for $\vec{\kappa}_- = -\frac{1}{2}$ and $\vec{\kappa}_+ = -2$ is shown in Figures 2. We observe that due to the choice of $\vec{\kappa}_\pm$, the phase $+1$ occupies the regions with smaller principal radius, while the phase -1 can be found where the membrane is rather flat. We show some more detail of the initial binodal decomposition in Figure 3.

We conducted the following shearing experiments on the domain $\Omega = (-2, 2)^2$ for an initial interface in the form of an ellipse, centred at the origin, with axis lengths 1 and 2.5. The length of the polygonal interface is 5.75, and it has 257 elements. For our choice of $\gamma = 0.05$ this yields on average about 7 elements across the interface. The time step size is $\tau = 5 \times 10^{-4}$. Once again we choose a random distribution for \mathfrak{C}^0 with mean value -0.4 . In particular, we prescribe the inhomogeneous Dirichlet boundary condition $\vec{g}(\vec{z}) = (z_2, 0)^T$ on $\partial_1\Omega = [-2, 2] \times \{\pm 2\}$. The remaining parameters are given by $\rho = \rho_\Gamma = 1$, $\alpha_- = 0.05$, $\alpha_+ = 0.2$ and either

$$(a) \quad \mu_+ = 1, \quad \mu_- = 1, \quad \text{or} \quad (b) \quad \mu_+ = 1, \quad \mu_- = 10. \quad (7.3)$$

The results can be seen in Figures 4 and 5, and they should be compared to the corresponding computations in the absence of any species effect, i.e. for $\mathfrak{C}^0 = -1$ constant, which can be seen in Figures 2 and 3 in Barrett et al. (2016a). As there, we observe tank treading when there is no viscosity contrast between inner and outer phase, and we observe tumbling when there is a viscosity contrast. The main difference to the computations in Barrett et al. (2016a), though, is that here the regions occupied by the $+1$ phase on the vesicle remain relatively straight throughout. This means that the tank treading motion in Figure 4 leads to concave shapes at times. Similarly, the phase distributions on the tumbling vesicle in Figure 5 have a notable effect on the vesicle shape, when compared with Figure 3 in Barrett et al. (2016a).

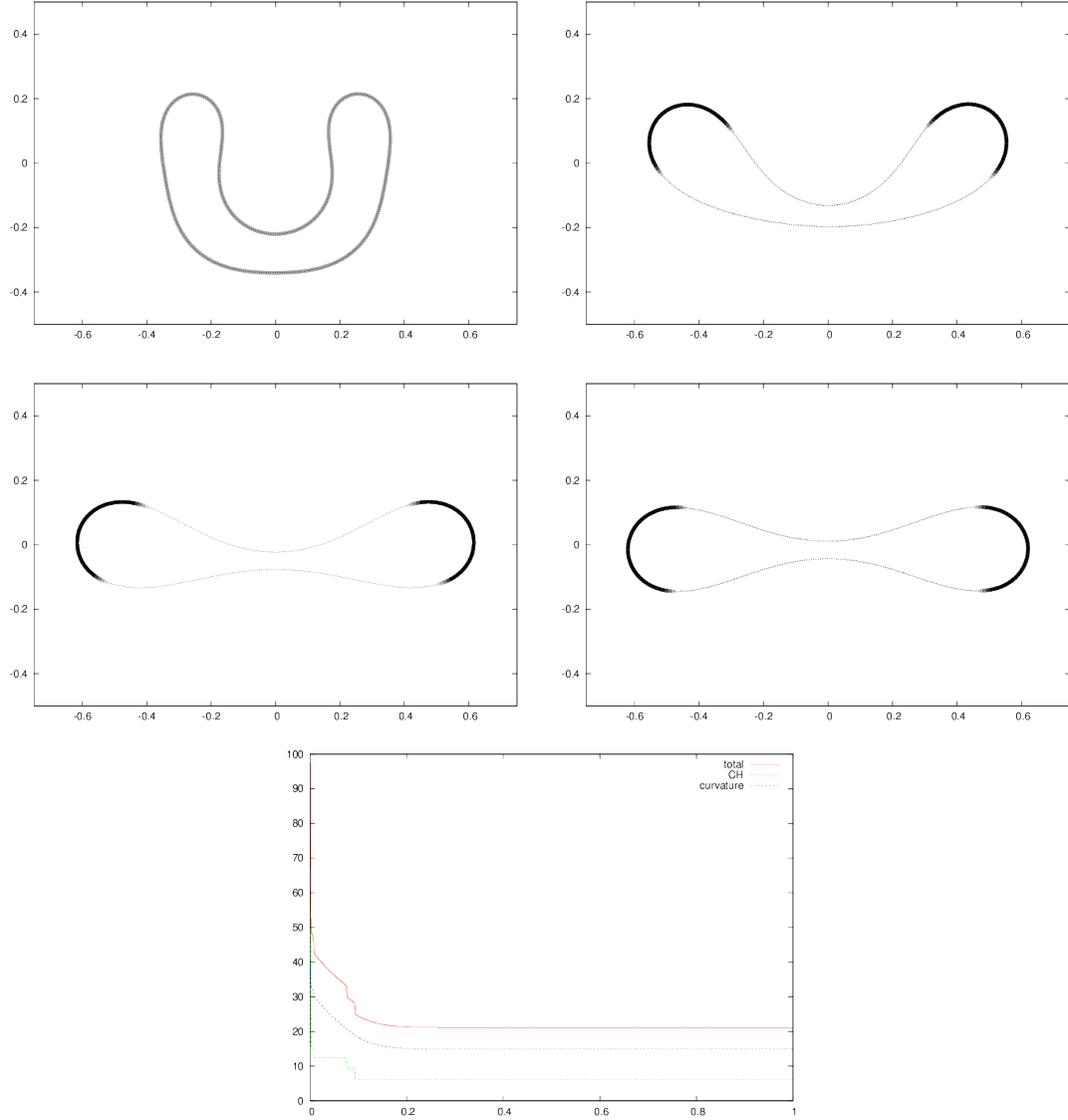


Figure 2: ($\alpha_{\pm} = 1$, $\overline{\alpha}_{-} = -\frac{1}{2}$, $\overline{\alpha}_{+} = -2$, $\beta = 1$) Flow for a smooth letter “C”. We show \mathfrak{C}^m on Γ^m at times $t = 0, 0.1, 0.2, 1$. Below a superimposed plot of the total discrete energy \mathcal{E}_{total}^h , the discrete Cahn–Hilliard energy, and the discrete curvature energy over $[0, 1]$.

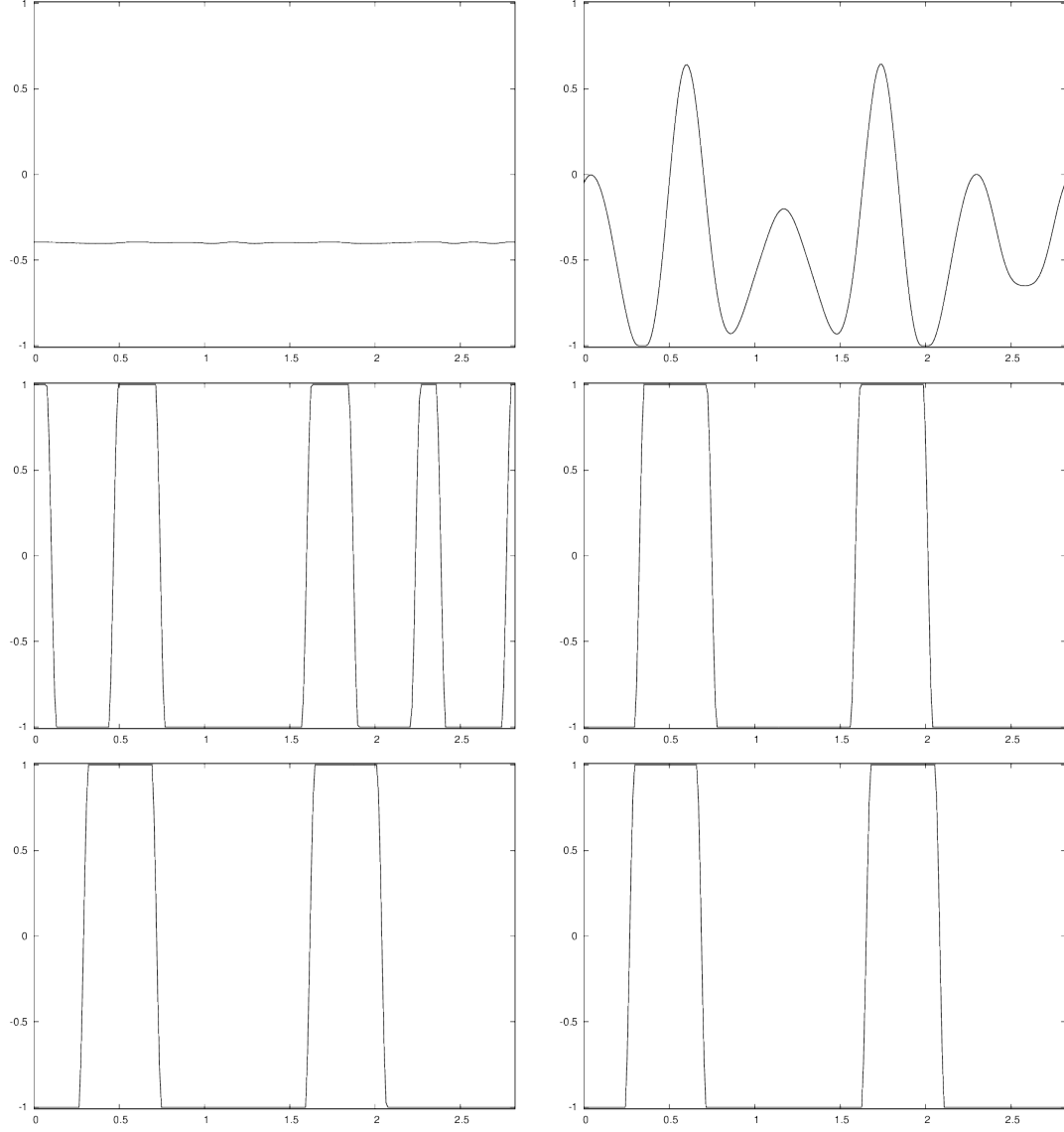


Figure 3: ($\alpha_{\pm} = 1$, $\overline{\alpha}_{-} = -\frac{1}{2}$, $\overline{\alpha}_{+} = -2$, $\beta = 1$) Flow for a smooth letter “C”. We show arclength plots of \mathfrak{C}^m at times $t = 0, 0.001, 0.01, 0.1, 0.2, 1$.

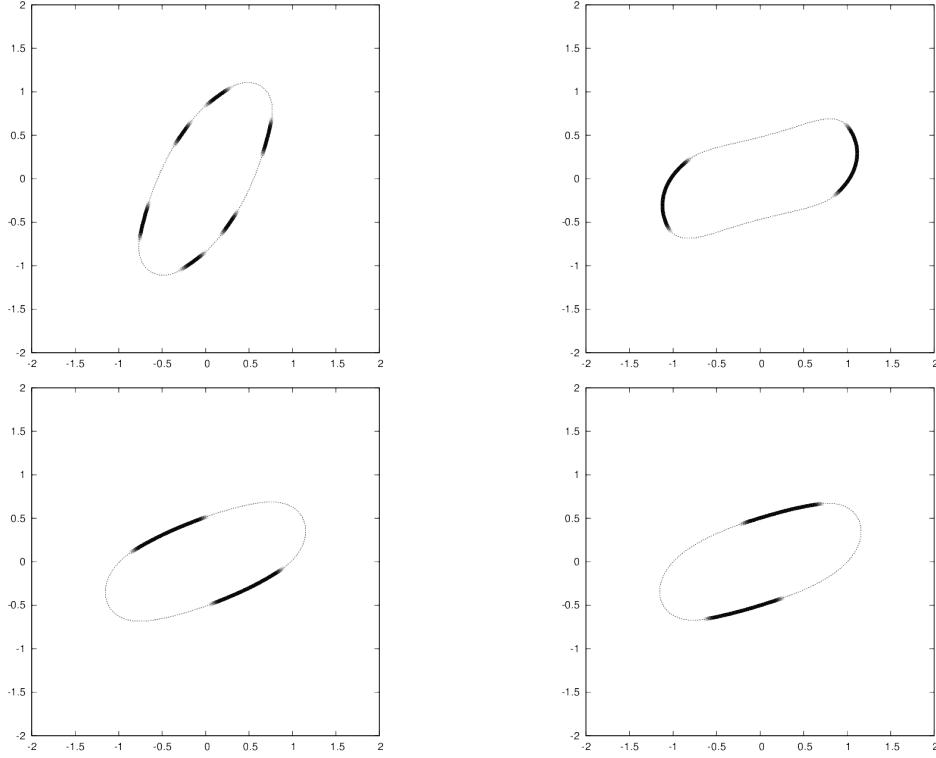


Figure 4: ($\alpha_- = 0.05$, $\alpha_+ = 0.2$, $\overline{\alpha}_\pm = 0$, $\beta = 1$) Shear flow with parameters as in (7.3a), leading to tank treading. The plots show the interface Γ^m , together with the concentration \mathfrak{C}^m at times $t = 1, 11, 13, 15$ (top left to bottom right).

Next we show a computation that highlights the Marangoni-type effects due to the tangential terms in (2.4). To this end, we start off with an initial interface that has an elliptic shape, on which the two phases are already well separated. The values of $\overline{\alpha}_\pm$ are then chosen such that a tangential movement of the phases leads to a decrease in energy. In particular, we let $\overline{\alpha}_- = 0.5$, $\overline{\alpha}_+ = 2$ and $\beta = 10$. The length of the polygonal interface is 5.75, and it has 257 elements. For our choice of $\gamma = 0.05$ this yields on average about 7 elements across the interface. The computational domain is $\Omega = (-2, 2)^2$, and the chosen time step size is $\tau = 5 \times 10^{-4}$. The results of the simulation are shown in Figure 6. It can be seen that due to the choice of $\overline{\alpha}_\pm$, the $+1$ phase moves away from an area of large convex bending to an area that is at first almost flat, and then settles on an area with a small concave bending. In Figure 7 we visualize the flow field for this computation, and compare it with a computation when $\mathfrak{C}^0 = 1$ constant, so that there are no tangential forces in (2.4). One clearly sees the effect of the tangential force which induces flow close to the interface also at later times.

On replacing the definition in (7.1a) with

$$\alpha(s) = s^2 \alpha_L(s) = \frac{1}{2} (\alpha_+ + \alpha_-) s^2 + \frac{1}{2} (\alpha_+ - \alpha_-) s^3, \quad (7.4a)$$

$$\text{or } \alpha(s) = (s^2 + \delta) \alpha_L(s), \quad \delta > 0, \quad (7.4b)$$

we can simulate C^0 -junctions, see also Helmers (2013), as long as $\delta \rightarrow 0$ for $\gamma \rightarrow 0$. We

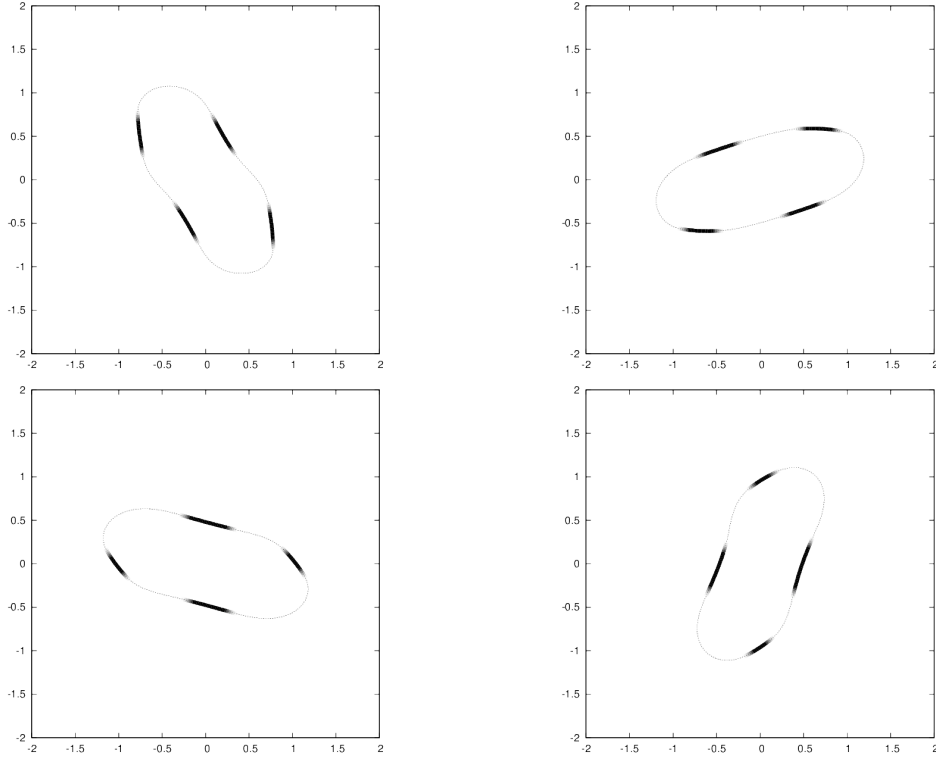


Figure 5: ($\alpha_- = 0.05$, $\alpha_+ = 0.2$, $\bar{\alpha}_\pm = 0$, $\beta = 1$) Shear flow with parameters as in (7.3b), leading to tumbling. The plots show the interface Γ^m , together with the concentration \mathfrak{C}^m at times $t = 8, 11, 14, 17$ (top left to bottom right).

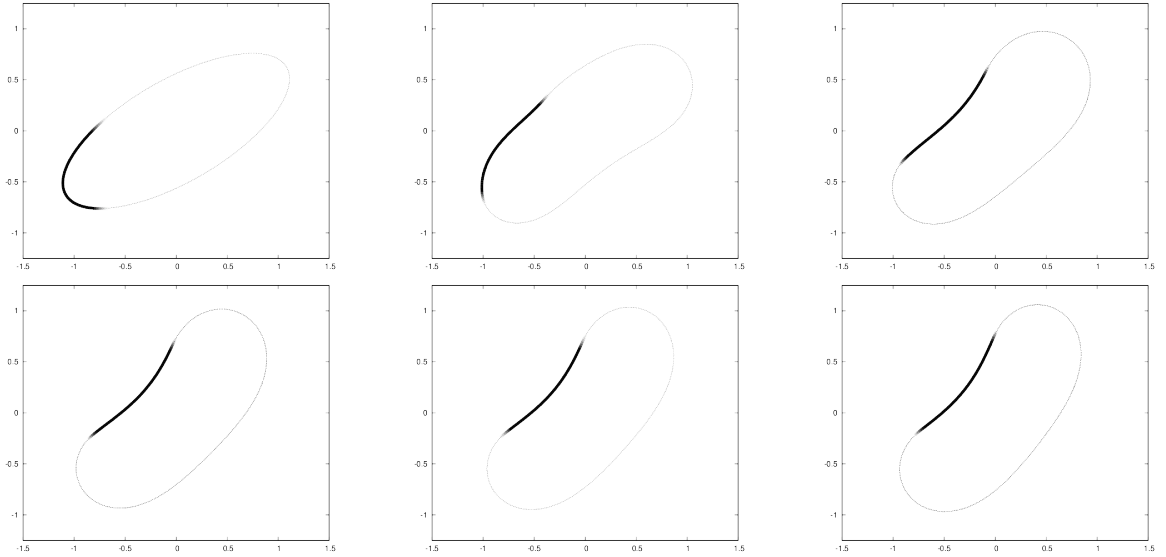


Figure 6: ($\alpha_\pm = 1$, $\bar{\alpha}_- = 0.5$, $\bar{\alpha}_+ = 2$, $\beta = 10$) Flow for an ellipse. We show \mathfrak{C}^m on Γ^m at times $t = 0, 1, 2, 3, 4, 10$.

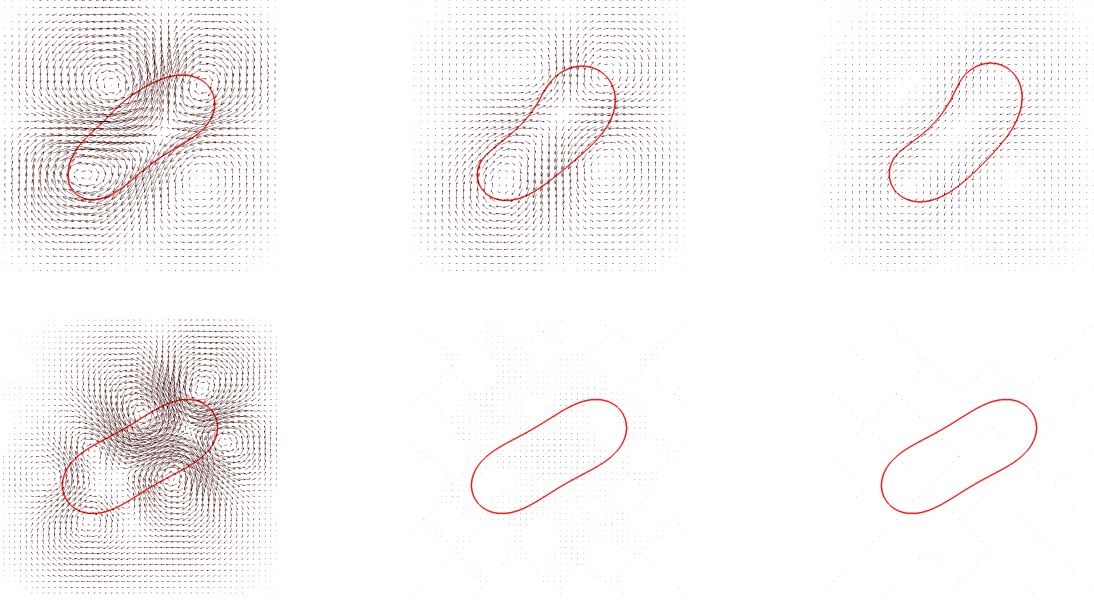


Figure 7: ($\alpha_{\pm} = 1$, $\bar{\kappa}_{-} = 0.5$, $\bar{\kappa}_{+} = 2$, $\beta = 10$) Visualization of the flow field \vec{U}^m at times $t = 1, 2, 3$ for the computation in Figure 6 (top), compared to the same computation with $\mathfrak{C}^m = 1$ constant throughout (bottom).

obtain interesting results starting from an ellipse, on which the two phases are already well separated, and using $\bar{\kappa}_{-} = -0.2$, $\bar{\kappa}_{+} = -2$ and $\beta = 10$. The length of the polygonal interface is 5.75, and it has 257 elements. For our choice of $\gamma = 0.05$ this yields on average about 7 elements across the interface. The computational domain is $\Omega = (-2, 2)^2$, and the chosen time step size is $\tau = 5 \times 10^{-4}$. In Figure 8 we show the numerical steady states for the two different evolutions. The nature of the C^0 -junction can clearly be seen, which allows for tangent discontinuities at the interface. This allows the $+1$ phase to reduce its contribution to the overall curvature energy. As a result, the total energy for the C^0 -steady state is 33.52, which is smaller than the value 33.97 for the C^1 -case. For the curvature energy contributions the comparison is 2.32 versus 2.83, again in favour of the C^0 -junction.

7.2 Numerical simulations in 3d

As a first example for a three-dimensional simulation, we consider the evolution for an initially flat plate of total dimension $4 \times 4 \times 1$, similarly to Barrett et al. (2016a, Fig. 8). The triangulations Γ^m satisfy $(K_{\Gamma}, J_{\Gamma}) = (1538, 3072)$, and the polygonal surfaces have a surface area of 35.7. This means that for our chosen value of $\gamma = 0.2$, there are on average about 5 elements across the interfacial region on Γ^m . As the computational domain we choose $\Omega = (-2.5, 2.5)^3$, and we use the time step size $\tau = 10^{-3}$. First we set $\alpha_{\pm} = 1$, $\bar{\kappa}_{\pm} = 0$ and $\beta = 1$, so that the only effect of the two phase aspect is given by the line energy contributions in the free energy. The initial distribution for \mathfrak{C}^0 is random

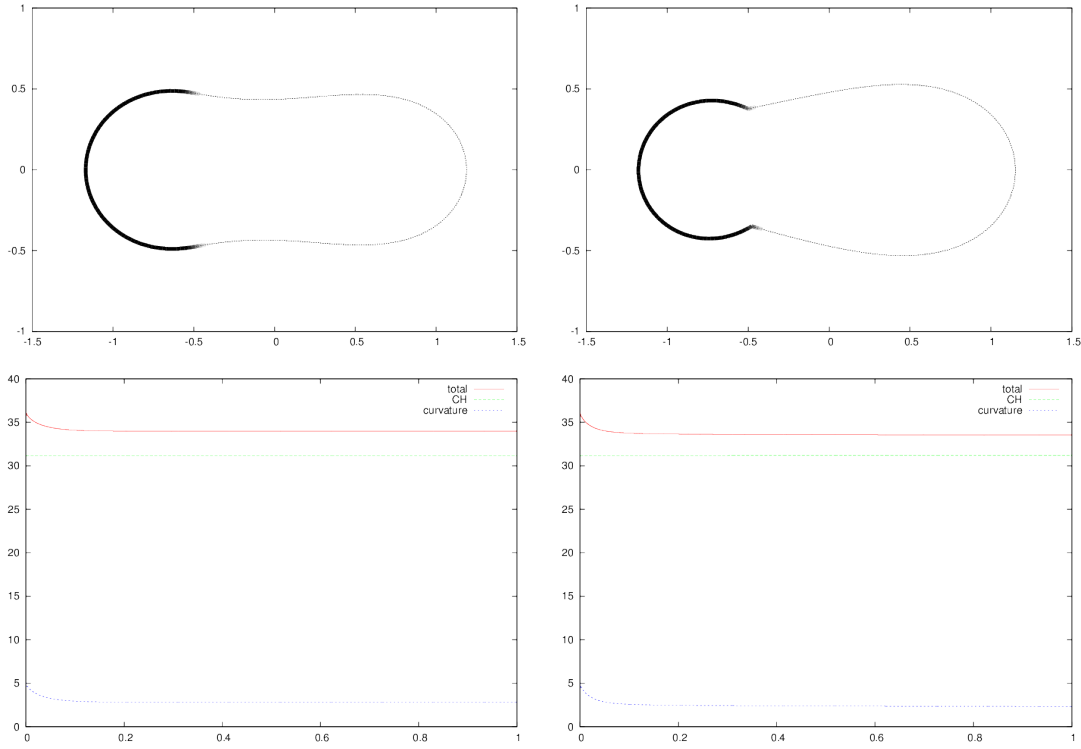


Figure 8: ($\alpha_{\pm} = 1$, $\bar{\alpha}_{-} = -0.2$, $\bar{\alpha}_{+} = -2$, $\beta = 10$) Solution at time $t = 1$ for the C^1 -case (left) and the C^0 -case (right). Below a superimposed plot of the total discrete energy \mathcal{E}_{total}^h , the discrete Cahn–Hilliard energy, and the discrete curvature energy over $[0, 1]$.

with mean value -0.4 . See Figure 9 for the evolution in this case. Repeating the same experiment for $\alpha_{-} = \frac{1}{2}$, $\alpha_{+} = 2$ gives the results in Figure 10. We note that the final shape is now a bit flatter, since the $+1$ phase does not allow the inner part of the membrane to become very concave.

In order to investigate budding, we start from a four-armed shape with well-developed interfaces between the two surface phases. As we use a finer mesh with $(K_{\Gamma}, J_{\Gamma}) = (3074, 6144)$, we now choose $\gamma = 0.1$. Moreover, we have set $\alpha_{\pm} = 1$, $\bar{\alpha}_{-} = -\frac{1}{2}$, $\bar{\alpha}_{+} = -2$ to encourage the forming of the buds. In the first experiment we set $\beta = 1$ and observe the results shown in Figure 11. The same experiment with $\beta = 5$ is shown in Figure 12, where we observe budding behaviour now. In particular, the $+1$ phase would like to pinch off the membrane at the four corners.

The numerical simulation of a vesicle flowing through a constriction can be seen in Figure 13. This is a two-phase analogue of the simulation shown in Barrett et al. (2016a, Figure 9). Here we choose the initial shape of the interface to be a biconcave surface resembling a human red blood cell. The shape has surface area 2.23, and the triangulations Γ^m satisfy $(K_{\Gamma}, J_{\Gamma}) = (3074, 6144)$. This means that for our chosen value of $\gamma = 0.05$, there are on average about 6 elements across the interfacial region on Γ^m . As the computational domain we choose $\Omega = (-2, -1) \times (-1, 1)^2 \cup [-1, 1] \times (-0.5, 0.5)^2 \cup (1, 2) \times (-1, 1)^2$. We define $\partial_2\Omega = \{2\} \times (-1, 1)^2$ and on $\partial_1\Omega$ we set no-slip conditions, except on the left

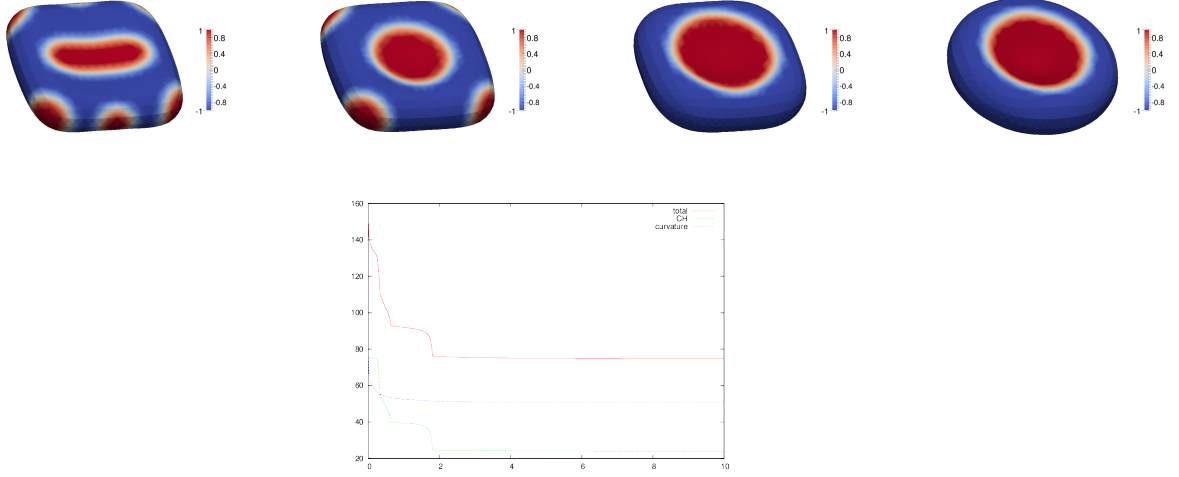


Figure 9: ($\alpha_{\pm} = 1$, $\overline{\alpha}_{\pm} = 0$, $\beta = 1$) Plots of \mathfrak{C}^m on Γ^m at times $t = 0.5, 1, 2, 10$. Below a superimposed plot of the total discrete energy \mathcal{E}_{total}^h , the discrete Cahn–Hilliard energy, and the discrete curvature energy over $[0, 10]$.

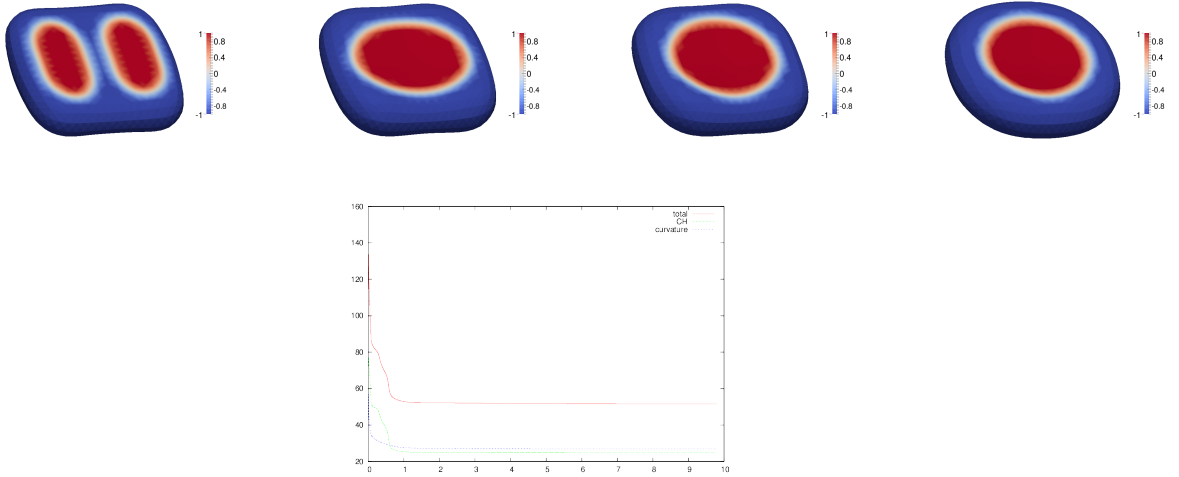


Figure 10: ($\alpha_- = \frac{1}{2}$, $\alpha_+ = 2$, $\overline{\alpha}_{\pm} = 0$, $\beta = 1$) Plots of \mathfrak{C}^m on Γ^m at times $t = 0.5, 1, 2, 10$. Compared to Figure 9, the final plot is less concave. Below a superimposed plot of the total discrete energy \mathcal{E}_{total}^h , the discrete Cahn–Hilliard energy, and the discrete curvature energy over $[0, 10]$.

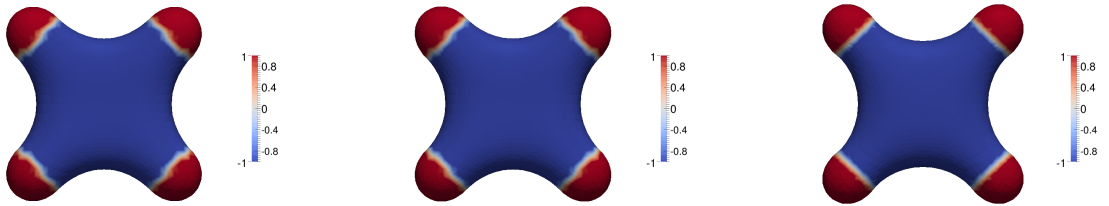


Figure 11: ($\alpha_{\pm} = 1$, $\overline{\alpha}_- = -\frac{1}{2}$, $\overline{\alpha}_+ = -2$, $\beta = 1$) Plots of \mathfrak{C}^m on Γ^m at times $t = 0.5, 1, 5$.

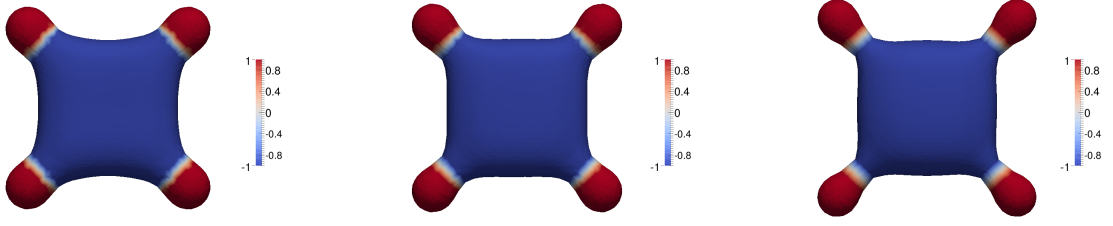


Figure 12: ($\alpha_{\pm} = 1$, $\overline{\alpha}_- = -\frac{1}{2}$, $\overline{\alpha}_+ = -2$, $\beta = 5$) Plots of \mathfrak{C}^m on Γ^m at times $t = 0.5, 1, 5$.

hand part $\{-2\} \times [-1, 1]^2$, where we prescribe the inhomogeneous boundary conditions $\vec{g}(\vec{z}) = ([1 - z_2^2 - z_3^2]_+, 0, 0)^T$ in order to model a Poiseuille-type flow. For the remaining parameters we set $\alpha_- = 0.05$, $\alpha_+ = 0.1$ and $\vartheta = 100$. We notice that during the evolution the membrane in Figure 13 deforms more than in the corresponding simulation with only a single phase $\mathfrak{C}^0 = 1$, see Barrett et al. (2016a, Figure 9). In particular, we observe that the $+1$ phase, which prefers a relatively flat surface, forces the surface to remain deformed also long after it has left the constriction.

In Figure 14 we show a numerical experiment for spinodal decomposition on a membrane, starting from a random distribution of phases with mean value -0.4 . The shape has surface area 35.7, and the triangulations Γ^m satisfy $(K_{\Gamma}, J_{\Gamma}) = (6146, 12288)$. This means that for our chosen value of $\gamma = 0.1$, there are on average about 6 elements across the interfacial region on Γ^m . Similarly, in Figure 15 we show the evolution for spinodal decomposition on a seven-arm surface, where the initial phase variable is $\mathfrak{C}^0 = -0.4$ constant. The shape has surface area 10.5, and the triangulations Γ^m satisfy $(K_{\Gamma}, J_{\Gamma}) = (2314, 4624)$. This means that for our chosen value of $\gamma = 0.2$, there are on average about 9 elements across the interfacial region on Γ^m . For the phase parameters we choose $\overline{\alpha}_- = -0.5$ and $\overline{\alpha}_+ = -2$. The spontaneous curvature of the $+1$ phase leads to a preference of the $+1$ phase to be curved away from the outer normal. In accordance with this remark we observe that the $+1$ phase appears after the phase separation at the more highly curved tips of the fingers.

In the following, we present some computations for $\alpha_{\pm}^G \neq 0$. When we repeat the experiment in Figure 9 for the choices $\alpha_-^G = 0.5$, $\alpha_+^G = 0$ and $\alpha_-^G = 0$, $\alpha_+^G = 0.5$, we obtain the results in Figures 16 and 17, respectively. We note that for this choice of parameters, the bound (7.2) holds. Comparing the results in Figure 9 with the ones in Figures 16 and 17 clearly shows the influence of the Gaussian energy terms. In Figure 16 the region of the largest Gaussian curvature is in the $+1$ phase and the region of the smallest Gaussian curvature is in the -1 phase. This is in accordance with the fact that the energy penalizes Gaussian curvature only in the -1 phase. On the other hand, in Figure 17 the region with the largest Gaussian curvature is the -1 phase and the $+1$ phase has a smaller Gaussian curvature when compared to Figure 16.

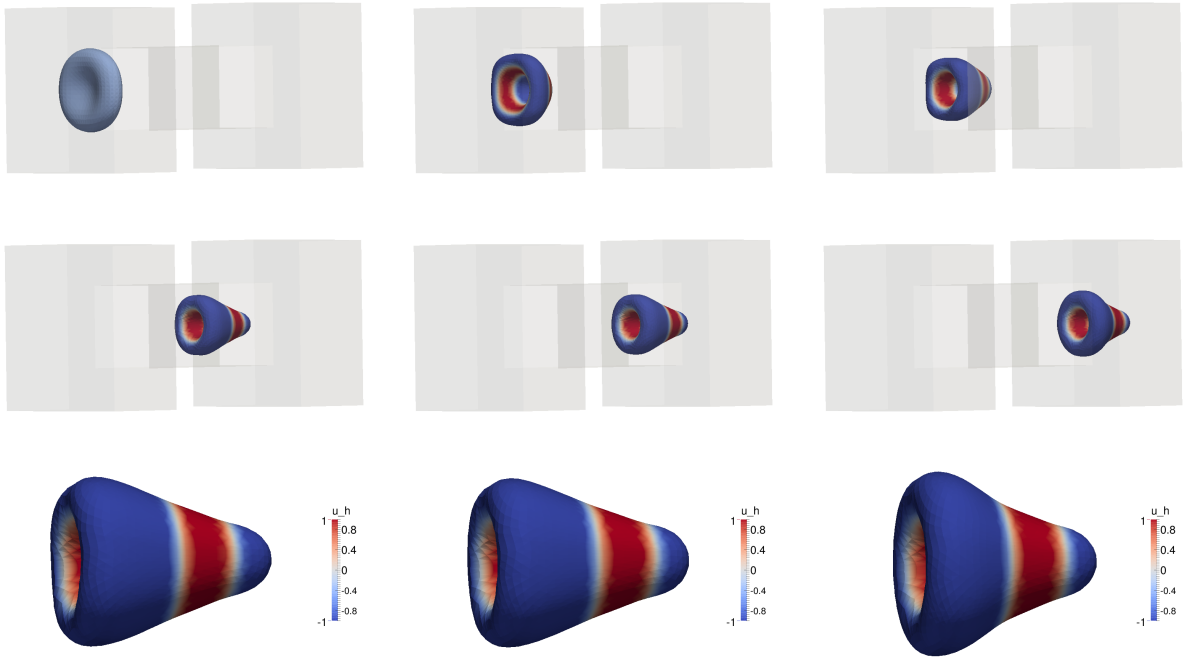


Figure 13: ($\alpha_- = 0.05$, $\alpha_+ = 0.1$, $\overline{\alpha}_{\pm} = 0$, $\beta = 1$, $\vartheta = 100$) Flow through a constriction. Plots of \mathfrak{C}^m on Γ^m at times $t = 0, 0.3, 0.5, 1, 1.2, 1.5$. Below we show enlarged plots of \mathfrak{C}^m on Γ^m at times $t = 1, 1.2, 1.5$.

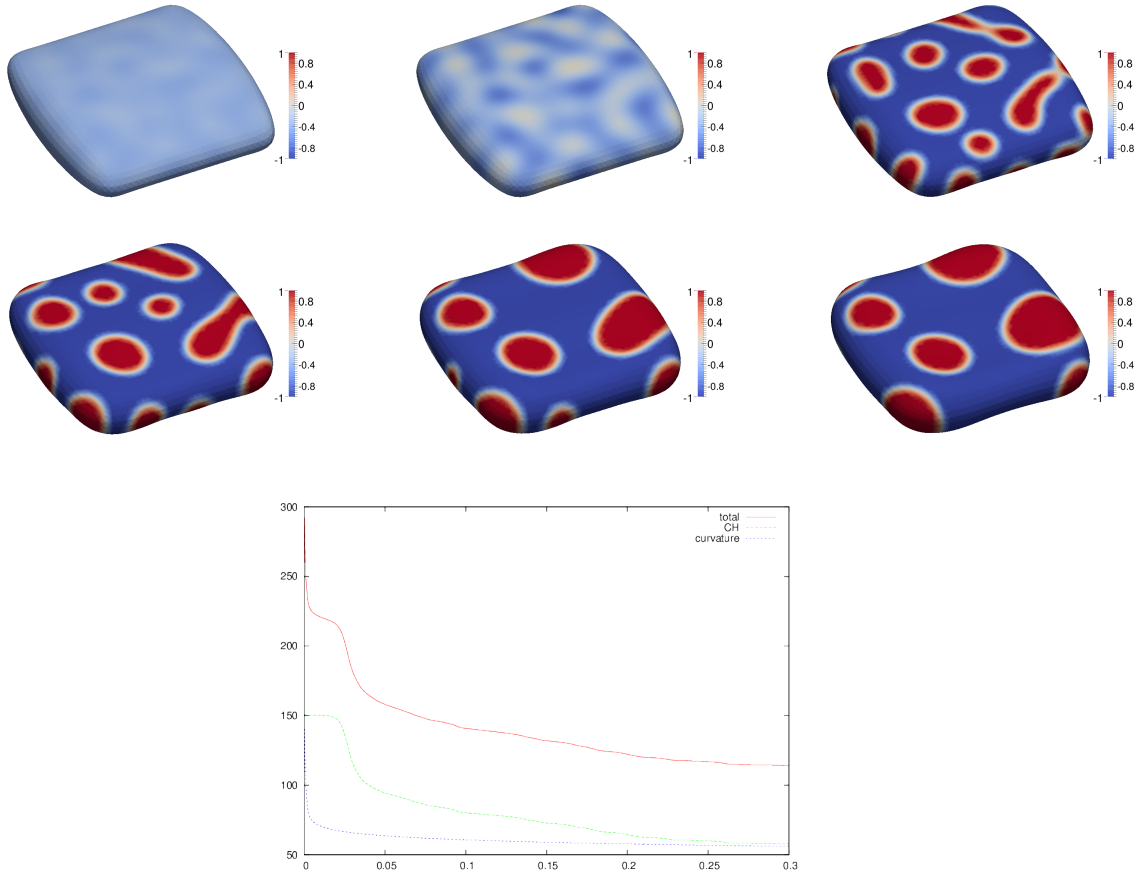


Figure 14: ($\alpha_{\pm} = 1$, $\overline{\alpha}_{\pm} = 0$, $\beta = 1$) Spinodal decomposition on a membrane. Plots of \mathfrak{C}^m on Γ^m at times $t = 0.01, 0.02, 0.05, 0.1, 0.2, 0.3$. Below a superimposed plot of the total discrete energy \mathcal{E}_{total}^h , the discrete Cahn–Hilliard energy, and the discrete curvature energy over $[0, 0.3]$.

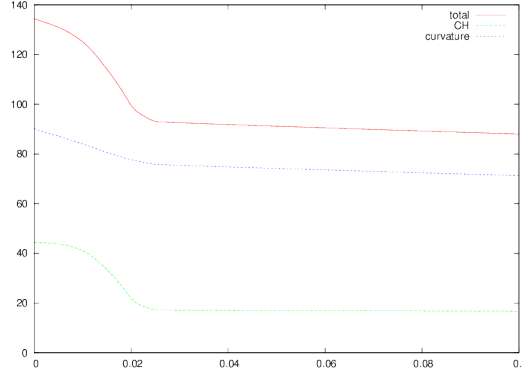
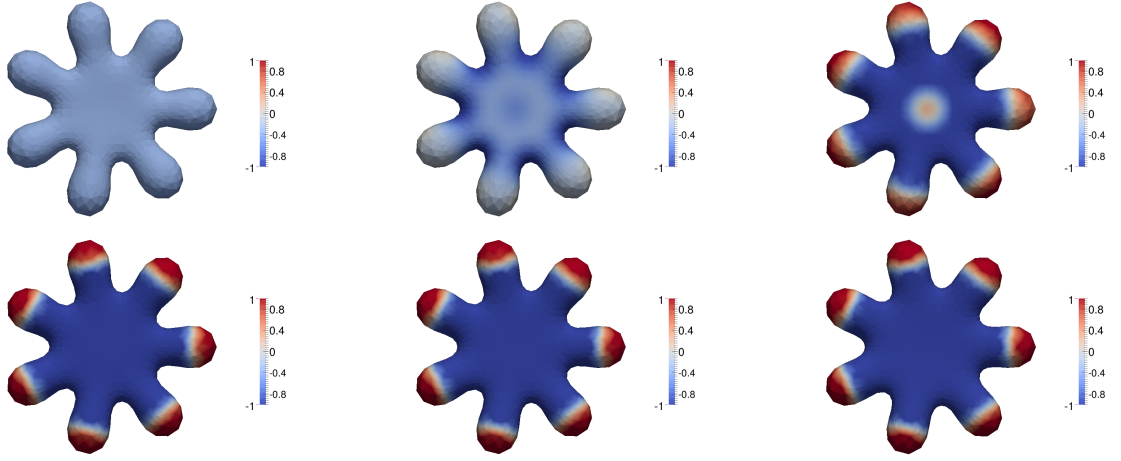


Figure 15: ($\alpha_{\pm} = 1$, $\overline{\alpha}_- = -0.5$, $\overline{\alpha}_+ = -2$, $\beta = 1$) Spinodal decomposition on a seven-arm membrane. Plots of \mathfrak{C}^m on Γ^m at times $t = 0, 0.01, 0.02, 0.03, 0.05, 0.1$. Below a superimposed plot of the total discrete energy \mathcal{E}_{total}^h , the discrete Cahn–Hilliard energy, and the discrete curvature energy over $[0, 0.1]$.

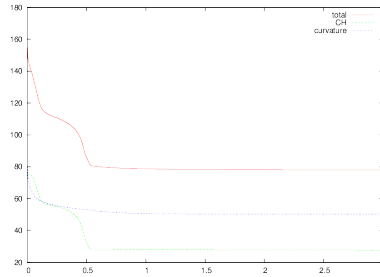
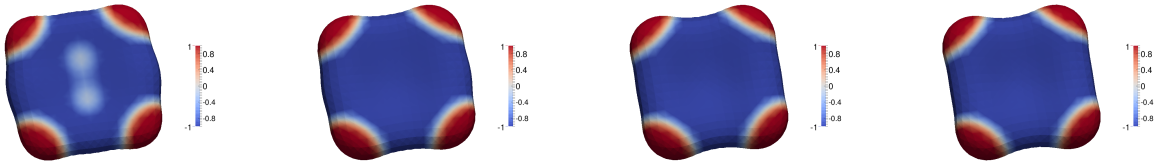


Figure 16: ($\alpha_{\pm} = 1$, $\overline{\alpha}_{\pm} = 0$, $\alpha_-^G = 0.5$, $\alpha_+^G = 0$, $\beta = 1$) Plots of \mathfrak{C}^m on Γ^m at times $t = 0.5, 1, 2, 3$. Below a superimposed plot of the total discrete energy \mathcal{E}_{total}^h , the discrete Cahn–Hilliard energy, and the discrete curvature energy over $[0, 3]$.

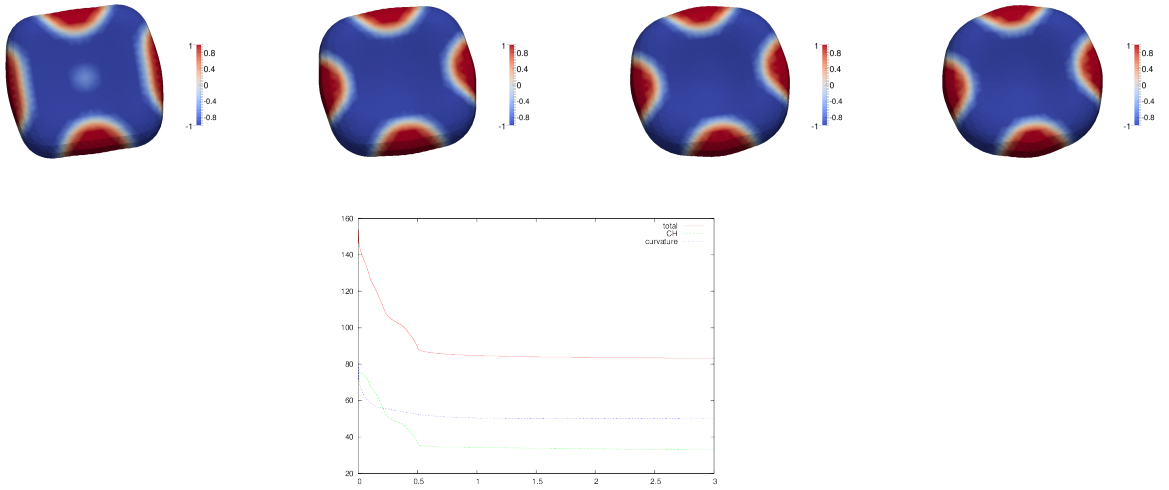


Figure 17: ($\alpha_{\pm} = 1$, $\bar{\alpha}_{\pm} = 0$, $\alpha_{-}^G = 0$, $\alpha_{+}^G = 0.5$, $\beta = 1$) Plots of \mathfrak{E}^m on Γ^m at times $t = 0.5, 1, 2, 3$. Below a superimposed plot of the total discrete energy \mathcal{E}_{total}^h , the discrete Cahn–Hilliard energy, and the discrete curvature energy over $[0, 3]$.

A Strong and weak formulations

The goal of this Appendix is to relate the weak formulation, (3.26a–e), (3.27b), of the first variations with respect to the geometry and \mathbf{c} of the energy in (1.2a), to the strong formulations (2.4) and (1.10b), respectively. As we allow for tangential motion, it is necessary to take into account variations which are not necessarily normal. This is in contrast to Elliott and Stinner (2010b), where only normal variations were considered.

We recall that $\nabla_s = (\partial_{s_1}, \dots, \partial_{s_d})^T$, and note from Dziuk and Elliott (2013, Lemma 2.6) that for sufficiently smooth ϕ it holds that

$$\partial_{s_k} \partial_{s_i} \phi - \partial_{s_i} \partial_{s_k} \phi = [(\nabla_s \vec{\nu}) \nabla_s \phi]_i \nu_k - [(\nabla_s \vec{\nu}) \nabla_s \phi]_k \nu_i \quad \forall i, k \in \{1, \dots, d\} \quad \text{on } \Gamma(t). \quad (\text{A.1})$$

It follows from (2.8), (A.1) and (2.9) that

$$\Delta_s \vec{\nu} = \nabla_s (\nabla_s \cdot \vec{\nu}) - |\nabla_s \vec{\nu}|^2 \vec{\nu} = -|\nabla_s \vec{\nu}|^2 \vec{\nu} - \nabla_s \boldsymbol{\kappa}. \quad (\text{A.2})$$

Moreover, we have from (2.9), (3.17), (3.14), (2.8), (3.16a) and (A.2) that

$$\begin{aligned} \partial_\varepsilon^0 \boldsymbol{\kappa} &= -\partial_\varepsilon^0 (\nabla_s \cdot \vec{\nu}) = -[\nabla_s \vec{\chi} - 2 \underline{\underline{D}}_s(\vec{\chi})] : \nabla_s \vec{\nu} - \nabla_s \cdot (\partial_\varepsilon^0 \vec{\nu}) \\ &= \nabla_s \vec{\chi} : \nabla_s \vec{\nu} + \nabla_s \cdot ([\nabla_s \vec{\chi}]^T \vec{\nu}) = 2 \nabla_s \vec{\chi} : \nabla_s \vec{\nu} + (\Delta_s \vec{\chi}) \cdot \vec{\nu} = \Delta_s (\vec{\chi} \cdot \vec{\nu}) - \vec{\chi} \cdot \Delta_s \vec{\nu} \\ &= \Delta_s (\vec{\chi} \cdot \vec{\nu}) + |\nabla_s \vec{\nu}|^2 (\vec{\chi} \cdot \vec{\nu}) + \vec{\chi} \cdot \nabla_s \boldsymbol{\kappa}. \end{aligned} \quad (\text{A.3})$$

A.1 Derivation of the strong formulation

We admit general variations $\vec{\chi} = \chi \vec{\nu} + \vec{\chi}_{\text{tan}}$, where $\vec{\chi}_{\text{tan}} \cdot \vec{\nu} = 0$, of (1.2a) with respect to Γ , whereas in Elliott and Stinner (2010b) only normal variations $\vec{\chi} = \chi \vec{\nu}$ of the geometry are considered.

We consider first the bending energy in (1.2a) and have from (3.12), on recalling (1.2b), that

$$\left[\frac{\delta}{\delta \Gamma} \langle b(\boldsymbol{\kappa}, \mathbf{c}), 1 \rangle_{\Gamma(t)} \right] (\vec{\chi}) = \langle \alpha(\mathbf{c}) (\boldsymbol{\kappa} - \overline{\boldsymbol{\kappa}}(\mathbf{c})), \partial_\varepsilon^0 \boldsymbol{\kappa} \rangle_{\Gamma(t)} + \langle b(\boldsymbol{\kappa}, \mathbf{c}), \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)}. \quad (\text{A.4})$$

We obtain from (A.4) and (A.3), on recalling (2.13), that

$$\begin{aligned} &\left[\frac{\delta}{\delta \Gamma} \langle b(\boldsymbol{\kappa}, \mathbf{c}), 1 \rangle_{\Gamma(t)} \right] (\vec{\chi}) \\ &= \langle \Delta_s [\alpha(\mathbf{c}) (\boldsymbol{\kappa} - \overline{\boldsymbol{\kappa}}(\mathbf{c}))] + \alpha(\mathbf{c}) [(\boldsymbol{\kappa} - \overline{\boldsymbol{\kappa}}(\mathbf{c})) |\nabla_s \vec{\nu}|^2 - \frac{1}{2} (\boldsymbol{\kappa} - \overline{\boldsymbol{\kappa}}(\mathbf{c}))^2 \boldsymbol{\kappa}], \vec{\chi} \cdot \vec{\nu} \rangle_{\Gamma(t)} \\ &\quad - \langle \nabla_s b(\boldsymbol{\kappa}, \mathbf{c}), \vec{\chi} \rangle_{\Gamma(t)} + \langle \alpha(\mathbf{c}) (\boldsymbol{\kappa} - \overline{\boldsymbol{\kappa}}(\mathbf{c})) \nabla_s \boldsymbol{\kappa}, \vec{\chi} \rangle_{\Gamma(t)} \\ &= \langle \Delta_s [\alpha(\mathbf{c}) (\boldsymbol{\kappa} - \overline{\boldsymbol{\kappa}}(\mathbf{c}))] + \alpha(\mathbf{c}) [(\boldsymbol{\kappa} - \overline{\boldsymbol{\kappa}}(\mathbf{c})) |\nabla_s \vec{\nu}|^2 - \frac{1}{2} (\boldsymbol{\kappa} - \overline{\boldsymbol{\kappa}}(\mathbf{c}))^2 \boldsymbol{\kappa}], \vec{\chi} \cdot \vec{\nu} \rangle_{\Gamma(t)} \\ &\quad - \langle b_{,\mathbf{c}}(\boldsymbol{\kappa}, \mathbf{c}), \vec{\chi} \cdot \nabla_s \mathbf{c} \rangle_{\Gamma(t)}. \end{aligned} \quad (\text{A.5a})$$

In addition, it holds that

$$\left[\frac{\delta}{\delta \mathbf{c}} \langle b(\boldsymbol{\varkappa}, \mathbf{c}), 1 \rangle_{\Gamma(t)} \right] (\eta) = \langle b_{,\mathbf{c}}(\boldsymbol{\varkappa}, \mathbf{c}), \eta \rangle_{\Gamma(t)}. \quad (\text{A.5b})$$

Choosing just a normal variation, $\vec{\chi} = \chi \vec{\nu}$, means that (A.5a,b) collapses to the result in Elliott and Stinner (2010b, (4.5)), on noting (2.5).

Next, we consider the interfacial energy in (1.2a). We have from (3.12), (3.19) and (2.13) that

$$\begin{aligned} \left[\frac{\delta}{\delta \Gamma} \langle b_{CH}(\mathbf{c}), 1 \rangle_{\Gamma(t)} \right] (\vec{\chi}) &= -\gamma \langle \nabla_s \mathbf{c}, (\nabla_s \vec{\chi}) \nabla_s \mathbf{c} \rangle_{\Gamma(t)} + \langle \tfrac{1}{2} \gamma |\nabla_s \mathbf{c}|^2 + \gamma^{-1} \Psi(\mathbf{c}), \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} \\ &= -\langle (\tfrac{1}{2} \gamma |\nabla_s \mathbf{c}|^2 + \gamma^{-1} \Psi(\mathbf{c})) \boldsymbol{\varkappa}, \vec{\chi} \cdot \vec{\nu} \rangle_{\Gamma(t)} - \langle \nabla_s (\tfrac{1}{2} \gamma |\nabla_s \mathbf{c}|^2 + \gamma^{-1} \Psi(\mathbf{c})), \vec{\chi} \rangle_{\Gamma(t)} \\ &\quad + \gamma \langle \nabla_s \cdot [(\nabla_s \mathbf{c}) \otimes (\nabla_s \mathbf{c})], \vec{\chi} \rangle_{\Gamma(t)}, \end{aligned} \quad (\text{A.6a})$$

where we have noted from (2.13) that

$$\langle \nabla_s \mathbf{c}, (\nabla_s \vec{\chi}) \nabla_s \mathbf{c} \rangle_{\Gamma(t)} = -\langle \nabla_s \cdot [(\nabla_s \mathbf{c}) \otimes (\nabla_s \mathbf{c})], \vec{\chi} \rangle_{\Gamma(t)}.$$

In addition, it holds that

$$\left[\frac{\delta}{\delta \mathbf{c}} \langle b_{CH}(\mathbf{c}), 1 \rangle_{\Gamma(t)} \right] (\eta) = \langle -\gamma \Delta_s \mathbf{c} + \gamma^{-1} \Psi'(\mathbf{c}), \eta \rangle_{\Gamma(t)}. \quad (\text{A.6b})$$

Once again, choosing a normal variation, $\vec{\chi} = \chi \vec{\nu}$, means that (A.6a,b) collapses to Elliott and Stinner (2010b, (4.8)), on noting that

$$\vec{\nu} \cdot (\nabla_s \cdot [(\nabla_s \mathbf{c}) \otimes (\nabla_s \mathbf{c})]) = -\nabla_s \vec{\nu} : [(\nabla_s \mathbf{c}) \otimes (\nabla_s \mathbf{c})].$$

For $d = 3$ only, we compute the first variation of the Gaussian curvature bending energy in (1.2a). We start by deriving an expression for $\partial_\varepsilon^0 \mathcal{K}$. On recalling (2.10), we first compute

$$\tfrac{1}{2} \partial_\varepsilon^0 |\nabla_s \vec{\nu}|^2 = \nabla_s \vec{\nu} : \partial_\varepsilon^0 (\nabla_s \vec{\nu}). \quad (\text{A.7})$$

From (3.18) we have that

$$\partial_\varepsilon^0 (\nabla_s \nu_i) = [\nabla_s \vec{\chi} - 2 \underline{\underline{D}}_s(\vec{\chi})] \nabla_s \nu_i + \nabla_s (\partial_\varepsilon^0 \nu_i) \quad i \in \{1, 2, 3\},$$

yielding, on noting (2.8) and (3.14), that

$$\begin{aligned} \partial_\varepsilon^0 (\nabla_s \vec{\nu}) &= \partial_\varepsilon^0 (\nabla_s \vec{\nu})^T = [\nabla_s \vec{\chi} - 2 \underline{\underline{D}}_s(\vec{\chi})] (\nabla_s \vec{\nu})^T + [\nabla_s (\partial_\varepsilon^0 \vec{\nu})]^T \\ &= [\nabla_s \vec{\chi} - 2 \underline{\underline{D}}_s(\vec{\chi})] \nabla_s \vec{\nu} + [\nabla_s ([\nabla_s \vec{\chi}]^T \vec{\nu})]^T. \end{aligned} \quad (\text{A.8})$$

We deduce from (A.7), (A.8), (2.8), (1.7b) and (3.16a) that

$$\tfrac{1}{2} \partial_\varepsilon^0 |\nabla_s \vec{\nu}|^2 = -\nabla_s \vec{\nu} : (\nabla_s \vec{\chi})^T \nabla_s \vec{\nu} - \nabla_s \vec{\nu} : \nabla_s ([\nabla_s \vec{\chi}]^T \vec{\nu}) = T_1 + T_2. \quad (\text{A.9})$$

Adopting the standard summation convention, we have that

$$T_1 = -(\partial_{s_j} \nu_i) (\partial_{s_k} \chi_i) \partial_{s_j} \nu_k = -(\partial_{s_i} \nu_k) (\partial_{s_j} \chi_k) \partial_{s_i} \nu_j = -(\partial_{s_k} \nu_i) (\partial_{s_j} \chi_k) \partial_{s_j} \nu_i \quad (\text{A.10})$$

and, on noting (2.8), that

$$\begin{aligned} T_2 &= -(\partial_{s_j} \nu_i) \partial_{s_j} ((\partial_{s_i} \chi_k) \nu_k) = -(\partial_{s_j} \nu_i) \partial_{s_j} (\partial_{s_i} (\chi_k \nu_k) - \chi_k \partial_{s_i} \nu_k) \\ &= -\partial_{s_j} ((\partial_{s_j} \nu_i) \partial_{s_i} (\chi_k \nu_k)) + (\partial_{s_j} \partial_{s_j} \nu_i) \partial_{s_i} (\chi_k \nu_k) + (\partial_{s_j} \nu_i) \partial_{s_j} (\chi_k \partial_{s_k} \nu_i) \\ &= -\partial_{s_j} ((\partial_{s_j} \nu_i) \partial_{s_i} (\chi_k \nu_k)) + (\partial_{s_j} \partial_{s_j} \nu_i) \partial_{s_i} (\chi_k \nu_k) \\ &\quad + (\partial_{s_j} \nu_i) [(\partial_{s_j} \partial_{s_k} \nu_i) \chi_k + (\partial_{s_j} \chi_k) \partial_{s_k} \nu_i] \\ &= -\nabla_s \cdot ((\nabla_s \vec{\nu}) \nabla_s (\vec{\chi} \cdot \vec{\nu})) + (\Delta_s \vec{\nu}) \cdot \nabla_s (\vec{\chi} \cdot \vec{\nu}) \\ &\quad + (\partial_{s_j} \nu_i) [(\partial_{s_j} \partial_{s_k} \nu_i) \chi_k + (\partial_{s_j} \chi_k) \partial_{s_k} \nu_i]. \end{aligned} \quad (\text{A.11})$$

Next, we note from (A.7) and (2.8) that

$$\begin{aligned} \chi_k (\partial_{s_j} \nu_i) (\partial_{s_j} \partial_{s_k} \nu_i) &= \chi_k (\partial_{s_j} \nu_i) [\partial_{s_k} \partial_{s_j} \nu_i - [(\nabla_s \vec{\nu}) \nabla_s \nu_i]_j \nu_k] \\ &= \frac{1}{2} \vec{\chi} \cdot \nabla_s |\nabla_s \vec{\nu}|^2 - ((\nabla_s \vec{\nu})^2 : \nabla_s \vec{\nu}) \vec{\chi} \cdot \vec{\nu}. \end{aligned} \quad (\text{A.12})$$

Combining (A.9)–(A.12) and noting (2.8) yields that

$$\begin{aligned} \frac{1}{2} \partial_\varepsilon^0 |\nabla_s \vec{\nu}|^2 &= -\nabla_s \cdot ((\nabla_s \vec{\nu}) \nabla_s (\vec{\chi} \cdot \vec{\nu})) + (\Delta_s \vec{\nu}) \cdot \nabla_s (\vec{\chi} \cdot \vec{\nu}) + \frac{1}{2} \vec{\chi} \cdot \nabla_s |\nabla_s \vec{\nu}|^2 \\ &\quad - \text{tr}((\nabla_s \vec{\nu})^3) \vec{\chi} \cdot \vec{\nu}. \end{aligned} \quad (\text{A.13})$$

As the eigenvalues of $-\nabla_s \vec{\nu}$ are 0, \varkappa_1 and \varkappa_2 , we have from (2.8) and (2.9) that

$$\begin{aligned} (\nabla_s \vec{\nu})^2 : (\nabla_s \vec{\nu}) &= \text{tr}((\nabla_s \vec{\nu})^3) = -(\varkappa_1^3 + \varkappa_2^3) = -(\varkappa_1^2 + \varkappa_2^2 - \varkappa_1 \varkappa_2) (\varkappa_1 + \varkappa_2) \\ &= (\mathcal{K} - |\nabla_s \vec{\nu}|^2) \varkappa. \end{aligned} \quad (\text{A.14})$$

Combining (A.13) and (A.14), on noting (A.2), yields that

$$\begin{aligned} \frac{1}{2} \partial_\varepsilon^0 |\nabla_s \vec{\nu}|^2 &= -\nabla_s \cdot ((\nabla_s \vec{\nu}) \nabla_s (\vec{\chi} \cdot \vec{\nu})) - (\nabla_s \varkappa) \cdot \nabla_s (\vec{\chi} \cdot \vec{\nu}) + \frac{1}{2} (\nabla_s |\nabla_s \vec{\nu}|^2) \cdot \vec{\chi} \\ &\quad + (|\nabla_s \vec{\nu}|^2 - \mathcal{K}) \varkappa \vec{\chi} \cdot \vec{\nu}. \end{aligned} \quad (\text{A.15})$$

On recalling (2.10) and (A.3), and combining with (A.15), we finally have that

$$\begin{aligned} \partial_\varepsilon^0 \mathcal{K} &= \frac{1}{2} \partial_\varepsilon^0 (\varkappa^2 - |\nabla_s \vec{\nu}|^2) = \varkappa \partial_\varepsilon^0 \varkappa - \frac{1}{2} \partial_\varepsilon^0 |\nabla_s \vec{\nu}|^2 \\ &= \varkappa [\Delta_s (\vec{\chi} \cdot \vec{\nu}) + |\nabla_s \vec{\nu}|^2 \vec{\chi} \cdot \vec{\nu} + \vec{\chi} \cdot \nabla_s \varkappa] + \nabla_s \cdot ((\nabla_s \vec{\nu}) \nabla_s (\vec{\chi} \cdot \vec{\nu})) \\ &\quad + (\nabla_s \varkappa) \cdot \nabla_s (\vec{\chi} \cdot \vec{\nu}) - \frac{1}{2} (\nabla_s |\nabla_s \vec{\nu}|^2) \cdot \vec{\chi} - (|\nabla_s \vec{\nu}|^2 - \mathcal{K}) \varkappa \vec{\chi} \cdot \vec{\nu} \\ &= \varkappa \Delta_s (\vec{\chi} \cdot \vec{\nu}) + \frac{1}{2} (\nabla_s \varkappa^2) \cdot \vec{\chi} - \frac{1}{2} (\nabla_s |\nabla_s \vec{\nu}|^2) \cdot \vec{\chi} + \nabla_s \cdot ((\nabla_s \vec{\nu}) \nabla_s (\vec{\chi} \cdot \vec{\nu})) \\ &\quad + (\nabla_s \varkappa) \cdot \nabla_s (\vec{\chi} \cdot \vec{\nu}) + \mathcal{K} \varkappa \vec{\chi} \cdot \vec{\nu} \\ &= \nabla_s \cdot [(\varkappa \underline{\text{Id}} + \nabla_s \vec{\nu}) \nabla_s (\vec{\chi} \cdot \vec{\nu})] + \nabla_s \mathcal{K} \cdot \vec{\chi} + \mathcal{K} \varkappa \vec{\chi} \cdot \vec{\nu}. \end{aligned} \quad (\text{A.16})$$

On noting (3.12), (2.13) and (A.16), we have that

$$\begin{aligned}
& \left[\frac{\delta}{\delta \Gamma} \langle \alpha^G(\mathbf{c}), \mathcal{K} \rangle_{\Gamma(t)} \right] (\vec{\chi}) \\
&= \langle \alpha^G(\mathbf{c}), \partial_\varepsilon^0 \mathcal{K} \rangle_{\Gamma(t)} + \langle \alpha^G(\mathbf{c}) \mathcal{K}, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} \\
&= - \langle \mathcal{K}, \vec{\chi} \cdot \nabla_s \alpha^G(\mathbf{c}) \rangle_{\Gamma(t)} + \langle \alpha^G(\mathbf{c}), \partial_\varepsilon^0 \mathcal{K} - \vec{\chi} \cdot \nabla_s \mathcal{K} - \varkappa \mathcal{K} \vec{\chi} \cdot \vec{\nu} \rangle_{\Gamma(t)} \\
&= - \langle \mathcal{K}, \vec{\chi} \cdot \nabla_s \alpha^G(\mathbf{c}) \rangle_{\Gamma(t)} + \langle \alpha^G(\mathbf{c}), \nabla_s \cdot [(\varkappa \underline{\text{Id}} + \nabla_s \vec{\nu}) \nabla_s (\vec{\chi} \cdot \vec{\nu})] \rangle_{\Gamma(t)} \\
&= - \langle \mathcal{K}, \vec{\chi} \cdot \nabla_s \alpha^G(\mathbf{c}) \rangle_{\Gamma(t)} + \langle \nabla_s \cdot [(\varkappa \underline{\text{Id}} + \nabla_s \vec{\nu}) \nabla_s \alpha^G(\mathbf{c})], \vec{\chi} \cdot \vec{\nu} \rangle_{\Gamma(t)}. \tag{A.17a}
\end{aligned}$$

In addition, it holds that

$$\left[\frac{\delta}{\delta \mathbf{c}} \langle \alpha^G(\mathbf{c}), \mathcal{K} \rangle_{\Gamma(t)} \right] (\eta) = \langle (\alpha^G)'(\mathbf{c}) \eta, \mathcal{K} \rangle_{\Gamma(t)}. \tag{A.17b}$$

Once again, (A.17a,b) collapses to Elliott and Stinner (2010b, (4.6)) if $\vec{\chi} = \chi \vec{\nu}$. Finally, the Cayley–Hamilton theorem applied to $-\nabla_s \vec{\nu}$ yields, on recalling (2.8), that

$$(\nabla_s \vec{\nu})^3 + \varkappa (\nabla_s \vec{\nu})^2 + \mathcal{K} \nabla_s \vec{\nu} = \underline{\underline{0}} \quad \Rightarrow \quad (\nabla_s \vec{\nu} + \varkappa \underline{\text{Id}}) \underline{\underline{\mathcal{P}}_\Gamma} = \mathcal{K} (-\nabla_s \vec{\nu})^{-1} \underline{\underline{\mathcal{P}}_\Gamma},$$

where we note that $(\nabla_s \vec{\nu})^{-1}$ is well-defined on the tangent space. With this identity it is possible to show that $\nabla_s \cdot [(\varkappa \underline{\text{Id}} + \nabla_s \vec{\nu}) \nabla_s \alpha^G(\mathbf{c})] = \hat{\Delta}_s \alpha^G(\mathbf{c})$, where $\hat{\Delta}_s$ is the second surface Laplacian used in the paper of Mercker et al. (2013) to derive the first variation of the Gaussian curvature bending energy. However, comparing our (2.4) and e.g. Lemma 5.1 in Mercker et al. (2013), there appears to be a sign discrepancy in the latter.

It follows from (A.5a,b), (A.6a,b), (A.17a,b) and (1.2a,b) that

$$\left[\frac{\delta}{\delta \Gamma} E(\Gamma(t), \mathbf{c}(t)) \right] (\vec{\chi}) = - \left\langle \vec{f}_\Gamma, \vec{\chi} \right\rangle_{\Gamma(t)} \tag{A.18a}$$

and

$$\left[\frac{\delta}{\delta \mathbf{c}} E(\Gamma(t), \mathbf{c}(t)) \right] (\eta) = \langle \mathbf{m}, \eta \rangle_{\Gamma(t)}, \tag{A.18b}$$

where \vec{f}_Γ and \mathbf{m} are defined in (2.4) and (1.10b), respectively.

A.2 Weak formulation equals strong formulation

Here we show that the weak formulation (3.26a–e), (3.27b) equals the strong formulation (2.4), (1.10b).

Recall from (3.25a) and (3.26a) that minus the first variation of the Lagrangian (3.24)

with respect to the geometry is given by

$$\begin{aligned}
\vec{f}_\Gamma &= - \left[\frac{\delta}{\delta \Gamma} L \right] (\vec{\chi}) \\
&= \langle \nabla_s \vec{y}, \nabla_s \vec{\chi} \rangle_{\Gamma(t)} + \langle \nabla_s \cdot \vec{y}, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} - 2 \left\langle (\nabla_s \vec{y})^T, \underline{\underline{D}}_s(\vec{\chi}) (\nabla_s \text{id})^T \right\rangle_{\Gamma(t)} \\
&\quad - \frac{1}{2} \left\langle [\alpha(\mathbf{c}) |\vec{\varkappa} - \overline{\varkappa}(\mathbf{c}) \vec{\nu}|^2 - 2(\vec{y} \cdot \vec{\varkappa})] \nabla_s \text{id}, \nabla_s \vec{\chi} \right\rangle_{\Gamma(t)} \\
&\quad - \langle \alpha(\mathbf{c}) (\vec{\varkappa} - \overline{\varkappa}(\mathbf{c}) \vec{\nu}) \overline{\varkappa}(\mathbf{c}), [\nabla_s \vec{\chi}]^T \vec{\nu} \rangle_{\Gamma(t)} \\
&\quad - \beta \left\langle \frac{1}{2} \gamma |\nabla_s \mathbf{c}|^2 + \gamma^{-1} \Psi(\mathbf{c}), \nabla_s \cdot \vec{\chi} \right\rangle_{\Gamma(t)} + \beta \gamma \langle (\nabla_s \mathbf{c}) \otimes (\nabla_s \mathbf{c}), \nabla_s \vec{\chi} \rangle_{\Gamma(t)} \\
&\quad - \frac{1}{2} \langle \alpha^G(\mathbf{c}) (|\vec{\varkappa}|^2 - |\underline{\underline{w}}|^2), \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} + \langle \underline{\underline{w}} : \underline{\underline{z}}, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} + \langle \vec{\nu} \cdot (\nabla_s \cdot \underline{\underline{z}}), \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} \\
&\quad + \langle \vec{\nu} \cdot (\underline{\underline{z}} \vec{\varkappa}), \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} \\
&\quad + \sum_{i=1}^d \left[\langle \nu_i \nabla_s \vec{z}_i, \nabla_s \vec{\chi} \rangle_{\Gamma(t)} - 2 \left\langle \nu_i (\nabla_s \vec{z}_i)^T, \underline{\underline{D}}_s(\vec{\chi}) (\nabla_s \text{id})^T \right\rangle_{\Gamma(t)} \right] \\
&\quad - \langle \underline{\underline{z}} \vec{\varkappa}, [\nabla_s \vec{\chi}]^T \vec{\nu} \rangle_{\Gamma(t)} - \langle \nabla_s \cdot \underline{\underline{z}}, [\nabla_s \vec{\chi}]^T \vec{\nu} \rangle_{\Gamma(t)} = \sum_{\ell=1}^{14} T_\ell
\end{aligned} \tag{A.19}$$

for $\vec{\chi} \in [H^1(\Gamma(t))]^d$.

On recalling Remark 3.2 and $\vec{\varkappa} = \varkappa \vec{\nu}$, we have that

$$\underline{\underline{z}} = -\alpha^G(\mathbf{c}) \underline{\underline{w}} = -\alpha^G(\mathbf{c}) \nabla_s \vec{\nu} \quad \Rightarrow \quad \vec{z}_i = \underline{\underline{z}} \vec{e}_i = -\alpha^G(\mathbf{c}) \nabla_s \nu_i = -\alpha^G(\mathbf{c}) \partial_{s_i} \vec{\nu}, \tag{A.20}$$

and so it follows that $\underline{\underline{z}} \vec{\varkappa} = \vec{0}$. Hence $T_{11} = T_{13} = 0$. Moreover, $\vec{\nu} \cdot [\nabla_s \vec{\chi}]^T \vec{\nu} = 0$, which implies that $T_5 = 0$. In addition, we recall from (3.26b) and $\underline{\underline{w}}^T \vec{\nu} = \underline{\underline{w}} \vec{\nu} = \vec{0}$ that

$$\vec{y} = y \vec{\nu} \quad \text{with} \quad y = \alpha(\mathbf{c}) (\varkappa - \overline{\varkappa}(\mathbf{c})) + \alpha^G(\mathbf{c}) \varkappa, \tag{A.21}$$

and so as $\nabla_s \cdot \vec{\nu} = -\varkappa$ it holds, on recalling (1.2b), (2.11) and (2.13), that

$$\begin{aligned}
\sum_{\ell \in \{2,4,8\}} T_\ell &= -\langle y \varkappa, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} + T_4 + T_8 = -\langle b(\varkappa, \mathbf{c}) + \alpha^G(\mathbf{c}) \mathcal{K}, \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} \\
&= \langle \nabla_s [b(\varkappa, \mathbf{c}) + \alpha^G(\mathbf{c}) \mathcal{K}], \vec{\chi} \rangle_{\Gamma(t)} + \langle [b(\varkappa, \mathbf{c}) + \alpha^G(\mathbf{c}) \mathcal{K}] \varkappa, \vec{\chi} \cdot \vec{\nu} \rangle_{\Gamma(t)}. \tag{A.22}
\end{aligned}$$

It also holds, on noting Barrett et al. (2016d, (A.22), (A.19)) and (3.16b), where we stress that the notation $\underline{\underline{D}}(\vec{\chi})$ there differs from $\underline{\underline{D}}_s(\vec{\chi})$ here by a factor 2 and by the absence of the projections $\underline{\underline{\mathcal{P}}}_\Gamma$, that

$$\begin{aligned}
\sum_{\ell \in \{1,3\}} T_\ell &= \langle \nabla_s (y \vec{\nu}), \nabla_s \vec{\chi} \rangle_{\Gamma(t)} - 2 \left\langle [\nabla_s (y \vec{\nu})]^T, \underline{\underline{D}}_s(\vec{\chi}) (\nabla_s \text{id})^T \right\rangle_{\Gamma(t)} \\
&= \langle \nabla_s (y \vec{\nu}), \nabla_s \vec{\chi} \rangle_{\Gamma(t)} - \langle [\nabla_s (y \vec{\nu})]^T, (\nabla_s \vec{\chi} + (\nabla_s \vec{\chi})^T) \underline{\underline{\mathcal{P}}}_\Gamma \rangle_{\Gamma(t)} \\
&= \langle \nabla_s (y \vec{\nu}), (\vec{\nu} \otimes \vec{\nu}) \nabla_s \vec{\chi} \rangle_{\Gamma(t)} - \langle y \nabla_s \vec{\nu}, \nabla_s \vec{\chi} \rangle_{\Gamma(t)} \\
&= \langle \nabla_s y, \nabla_s (\vec{\chi} \cdot \vec{\nu}) \rangle_{\Gamma(t)} - \langle \nabla_s \cdot [y (\nabla_s \vec{\nu})^T \vec{\chi}], 1 \rangle_{\Gamma(t)} - \langle y (|\nabla_s \vec{\nu}|^2 \vec{\nu} + \nabla_s \varkappa), \vec{\chi} \rangle_{\Gamma(t)} \\
&= \langle \nabla_s y, \nabla_s (\vec{\chi} \cdot \vec{\nu}) \rangle_{\Gamma(t)} - \langle y (|\nabla_s \vec{\nu}|^2 \vec{\nu} + \nabla_s \varkappa), \vec{\chi} \rangle_{\Gamma(t)}, \tag{A.23}
\end{aligned}$$

where in the last equality we have noted that $\Gamma(t)$ is a closed surface. Moreover, we note from (A.21) and (1.2b) that

$$\begin{aligned} y \nabla_s \mathbf{x} &= [\alpha(\mathbf{c}) (\mathbf{x} - \overline{\mathbf{x}}(\mathbf{c})) + \alpha^G(\mathbf{c}) \mathbf{x}] \nabla_s \mathbf{x} \\ &= \nabla_s (b(\mathbf{x}, \mathbf{c}) + \frac{1}{2} \alpha^G(\mathbf{c}) \mathbf{x}^2) - [b_{,\mathbf{c}}(\mathbf{x}, \mathbf{c}) + \frac{1}{2} (\alpha^G)'(\mathbf{c}) \mathbf{x}^2] \nabla_s \mathbf{c}. \end{aligned} \quad (\text{A.24})$$

Combining (A.22), (A.23) and (A.24) yields, on noting (2.13), (A.21) and (2.11), that

$$\begin{aligned} \sum_{\ell \in \{1, \dots, 4, 8\}} T_\ell &= - \langle \Delta_s [\alpha(\mathbf{c}) (\mathbf{x} - \overline{\mathbf{x}}(\mathbf{c})) + \alpha^G(\mathbf{c}) \mathbf{x}], \vec{\chi} \cdot \vec{\nu} \rangle_{\Gamma(t)} \\ &\quad + \langle [b(\mathbf{x}, \mathbf{c}) + \alpha^G(\mathbf{c}) \mathcal{K}] \mathbf{x}, \vec{\chi} \cdot \vec{\nu} \rangle_{\Gamma(t)} + \langle [b_{,\mathbf{c}}(\mathbf{x}, \mathbf{c}) + \frac{1}{2} (\alpha^G)'(\mathbf{c}) \mathbf{x}^2] \nabla_s \mathbf{c}, \vec{\chi} \rangle_{\Gamma(t)} \\ &\quad - \langle (\alpha(\mathbf{c}) (\mathbf{x} - \overline{\mathbf{x}}(\mathbf{c})) + \alpha^G(\mathbf{c}) \mathbf{x}) |\nabla_s \vec{\nu}|^2, \vec{\chi} \cdot \vec{\nu} \rangle_{\Gamma(t)} \\ &\quad - \frac{1}{2} \langle \nabla_s (\alpha^G(\mathbf{c}) |\nabla_s \vec{\nu}|^2), \vec{\chi} \rangle_{\Gamma(t)}. \end{aligned} \quad (\text{A.25})$$

It holds on noting (2.13) that

$$\begin{aligned} \sum_{\ell \in \{6, 7\}} T_\ell &= \beta \langle \nabla_s [\frac{1}{2} \gamma |\nabla_s \mathbf{c}|^2 + \gamma^{-1} \Psi(\mathbf{c})], \vec{\chi} \rangle_{\Gamma(t)} + \beta \langle [\frac{1}{2} \gamma |\nabla_s \mathbf{c}|^2 + \gamma^{-1} \Psi(\mathbf{c})] \mathbf{x}, \vec{\chi} \cdot \vec{\nu} \rangle_{\Gamma(t)} \\ &\quad - \beta \gamma \langle \nabla_s \cdot ((\nabla_s \mathbf{c}) \otimes (\nabla_s \mathbf{c})), \vec{\chi} \rangle_{\Gamma(t)}. \end{aligned} \quad (\text{A.26})$$

In addition, we have from (A.20) that

$$\begin{aligned} \sum_{\ell \in \{9, 10\}} T_\ell &= \langle \underline{w} : \underline{z} + \vec{\nu} \cdot (\nabla_s \cdot \underline{z}), \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} \\ &= - \langle \alpha^G(\mathbf{c}) |\nabla_s \vec{\nu}|^2 + \vec{\nu} \cdot [\nabla_s \cdot (\alpha^G(\mathbf{c}) \nabla_s \vec{\nu})], \nabla_s \cdot \vec{\chi} \rangle_{\Gamma(t)} = 0, \end{aligned} \quad (\text{A.27})$$

where we have observed from (A.2) that

$$\begin{aligned} \vec{\nu} \cdot [\nabla_s \cdot (\alpha^G(\mathbf{c}) \nabla_s \vec{\nu})] &= \vec{\nu} \cdot [\alpha^G(\mathbf{c}) \Delta_s \vec{\nu} + (\nabla_s \vec{\nu}) \nabla_s \alpha^G(\mathbf{c})] = \alpha^G(\mathbf{c}) \vec{\nu} \cdot \Delta_s \vec{\nu} \\ &= \alpha^G(\mathbf{c}) \vec{\nu} \cdot [-|\nabla_s \vec{\nu}|^2 \vec{\nu} - \nabla_s \mathbf{x}] = -\alpha^G(\mathbf{c}) |\nabla_s \vec{\nu}|^2. \end{aligned} \quad (\text{A.28})$$

It follows from (3.16b) and $\underline{\mathcal{P}}_\Gamma = \nabla_s \text{id}$ that

$$\begin{aligned} T_{12} &= \sum_{i=1}^d \left[\langle \nu_i \nabla_s \vec{z}_i, \nabla_s \vec{\chi} \rangle_{\Gamma(t)} - 2 \left\langle \nu_i (\nabla_s \vec{z}_i)^T, \underline{\mathcal{D}}_s(\vec{\chi}) (\nabla_s \text{id})^T \right\rangle_{\Gamma(t)} \right] \\ &= - \sum_{i=1}^d \langle \nu_i (\nabla_s \vec{z}_i)^T, \nabla_s \vec{\chi} \rangle_{\Gamma(t)}, \end{aligned} \quad (\text{A.29})$$

provided that we can show that

$$\sum_{i=1}^d \left[\langle \nu_i \nabla_s \vec{z}_i, \nabla_s \vec{\chi} \rangle_{\Gamma(t)} - \langle \nu_i (\nabla_s \vec{z}_i)^T, (\nabla_s \vec{\chi})^T \underline{\mathcal{P}}_\Gamma \rangle_{\Gamma(t)} \right] = 0. \quad (\text{A.30})$$

In order to establish (A.30), we note, on recalling (A.20) and (A.1), that

$$\begin{aligned}
\nu_i \nabla_s \vec{z}_i : \nabla_s \vec{\chi} - \nu_i (\nabla_s \vec{z}_i)^T : [(\nabla_s \vec{\chi})^T \underline{\mathcal{P}}_\Gamma] &= \nu_i (\nabla_s \vec{z}_i)_{kj} [\partial_{s_j} \chi_k - (\partial_{s_j} \chi_l) (\delta_{lk} - \nu_l \nu_k)] \\
&= \nu_i (\nabla_s \vec{z}_i)_{kj} (\partial_{s_j} \chi_l) \nu_l \nu_k = -\nu_i [\partial_{s_j} (\alpha^G(\mathbf{c}) \partial_{s_k} \nu_i)] (\partial_{s_j} \chi_l) \nu_l \nu_k \\
&= -\nu_i \nu_l \nu_k \alpha^G(\mathbf{c}) (\partial_{s_j} \partial_{s_k} \nu_i) \partial_{s_j} \chi_l = \nu_i \nu_l \nu_k \alpha^G(\mathbf{c}) [(\nabla_s \vec{\nu}) \nabla_s \nu_i]_j \nu_k \partial_{s_j} \chi_l \\
&= \nu_i \nu_l \alpha^G(\mathbf{c}) [(\nabla_s \vec{\nu}) \nabla_s \nu_i]_j \partial_{s_j} \chi_l = \nu_i \nu_l \alpha^G(\mathbf{c}) (\partial_{s_k} \nu_j) (\partial_{s_k} \nu_i) \partial_{s_j} \chi_l = 0, \quad (\text{A.31})
\end{aligned}$$

since $\nu_i \partial_{s_k} \nu_i = \frac{1}{2} \partial_{s_k} |\vec{\nu}|^2 = 0$.

Returning to (A.29), we have on noting (A.20), (2.13), (A.1) and (A.2) that

$$\begin{aligned}
T_{12} &= - \sum_{i=1}^d \langle \nu_i \nabla_s \vec{z}_i, (\nabla_s \vec{\chi})^T \rangle_{\Gamma(t)} = \langle \nu_i \partial_{s_l} (\alpha^G(\mathbf{c}) \partial_{s_k} \nu_i), \partial_{s_k} \chi_l \rangle_{\Gamma(t)} \\
&= \langle \alpha^G(\mathbf{c}) \nu_i \partial_{s_l} \partial_{s_k} \nu_i, \partial_{s_k} \chi_l \rangle_{\Gamma(t)} = - \langle \alpha^G(\mathbf{c}) (\partial_{s_l} \nu_i) \partial_{s_k} \nu_i, \partial_{s_k} \chi_l \rangle_{\Gamma(t)} \\
&= \langle \alpha^G(\mathbf{c}) [(\partial_{s_k} \partial_{s_l} \nu_i) \partial_{s_k} \nu_i + (\partial_{s_l} \nu_i) \partial_{s_k} \partial_{s_k} \nu_i] + (\partial_{s_k} \alpha^G(\mathbf{c})) (\partial_{s_l} \nu_i) \partial_{s_k} \nu_i, \chi_l \rangle_{\Gamma(t)} \\
&= \langle \alpha^G(\mathbf{c}) \partial_{s_k} \nu_i [\partial_{s_l} \partial_{s_k} \nu_i - [(\nabla_s \vec{\nu}) \nabla_s \nu_i]_k \nu_l], \chi_l \rangle_{\Gamma(t)} - \langle \alpha^G(\mathbf{c}) (\partial_{s_l} \nu_i) \partial_{s_i} \nu_l, \chi_l \rangle_{\Gamma(t)} \\
&\quad + \langle (\partial_{s_k} \alpha^G(\mathbf{c})) (\partial_{s_l} \nu_i) \partial_{s_k} \nu_i, \chi_l \rangle_{\Gamma(t)} \\
&= \frac{1}{2} \langle \alpha^G(\mathbf{c}) \nabla_s |\nabla_s \vec{\nu}|^2, \vec{\chi} \rangle_{\Gamma(t)} - \langle \alpha^G(\mathbf{c}) (\nabla_s \vec{\nu})^2, \nabla_s \vec{\nu} (\vec{\chi} \cdot \vec{\nu}) \rangle_{\Gamma(t)} \\
&\quad - \langle \alpha^G(\mathbf{c}) (\nabla_s \vec{\nu}) \nabla_s \nu_l, \vec{\chi} \rangle_{\Gamma(t)} + \langle (\nabla_s \vec{\nu})^2 \nabla_s \alpha^G(\mathbf{c}), \vec{\chi} \rangle_{\Gamma(t)}. \quad (\text{A.32})
\end{aligned}$$

The remaining term from (A.19) can be rewritten, on noting (A.20), (2.13), (A.2) and (2.8), as

$$\begin{aligned}
T_{14} &= - \sum_{i=1}^d \langle (\partial_{s_i} \vec{z}_i) \otimes \vec{\nu}, (\nabla_s \vec{\chi})^T \rangle_{\Gamma(t)} \\
&= \langle \partial_{s_i} (\alpha^G(\mathbf{c}) \partial_{s_i} \nu_k), \nu_l \partial_{s_k} \chi_l \rangle_{\Gamma(t)} \\
&= \langle (\partial_{s_i} \alpha^G(\mathbf{c})) \partial_{s_i} \nu_k + \alpha^G(\mathbf{c}) \partial_{s_i} \partial_{s_i} \nu_k, \nu_l \partial_{s_k} \chi_l \rangle_{\Gamma(t)} \\
&= \langle (\partial_{s_i} \alpha^G(\mathbf{c})) \partial_{s_i} \nu_k - \alpha^G(\mathbf{c}) \partial_{s_k} \nu_l, \nu_l \partial_{s_k} \chi_l \rangle_{\Gamma(t)} \\
&= - \langle (\partial_{s_k} [(\partial_{s_i} \alpha^G(\mathbf{c})) \partial_{s_i} \nu_k]) \nu_l + (\partial_{s_i} \alpha^G(\mathbf{c})) (\partial_{s_i} \nu_k) \partial_{s_k} \nu_l, \chi_l \rangle_{\Gamma(t)} \\
&\quad - \langle (\partial_{s_i} \alpha^G(\mathbf{c})) (\partial_{s_k} \nu_i) \nu_l, \chi_l \rangle_{\Gamma(t)} \\
&\quad + \langle (\partial_{s_k} [\alpha^G(\mathbf{c}) \partial_{s_k} \nu_l]) \nu_i + \alpha^G(\mathbf{c}) (\partial_{s_k} \nu_l) \partial_{s_k} \nu_i, \chi_l \rangle_{\Gamma(t)} \\
&= - \langle \nabla_s \cdot [(\nabla_s \vec{\nu}) \nabla_s \alpha^G(\mathbf{c})], \vec{\chi} \cdot \vec{\nu} \rangle_{\Gamma(t)} - \langle (\nabla_s \vec{\nu})^2 \nabla_s \alpha^G(\mathbf{c}), \vec{\chi} \rangle_{\Gamma(t)} \\
&\quad + \langle \nabla_s \cdot (\alpha^G(\mathbf{c}) \nabla_s \nu_l), \vec{\chi} \cdot \vec{\nu} \rangle_{\Gamma(t)} + \langle \alpha^G(\mathbf{c}) (\nabla_s \vec{\nu}) \nabla_s \nu_l, \vec{\chi} \rangle_{\Gamma(t)}. \quad (\text{A.33})
\end{aligned}$$

Hence we have from (A.32) and (A.33), on noting (A.14) for $d = 3$ and on recalling that $\alpha^G = 0$ for $d = 2$, that

$$\begin{aligned}
\sum_{\ell \in \{12, 14\}} T_\ell &= \frac{1}{2} \langle \alpha^G(\mathbf{c}) \nabla_s |\nabla_s \vec{\nu}|^2, \vec{\chi} \rangle_{\Gamma(t)} + \langle \alpha^G(\mathbf{c}) [|\nabla_s \vec{\nu}|^2 - \mathcal{K}] \nu_l, \vec{\chi} \cdot \vec{\nu} \rangle_{\Gamma(t)} \\
&\quad - \langle \nabla_s \cdot [(\nabla_s \vec{\nu}) \nabla_s \alpha^G(\mathbf{c})], \vec{\chi} \cdot \vec{\nu} \rangle_{\Gamma(t)} + \langle \nabla_s \cdot [\alpha^G(\mathbf{c}) \nabla_s \nu_l], \vec{\chi} \cdot \vec{\nu} \rangle_{\Gamma(t)}. \quad (\text{A.34})
\end{aligned}$$

Combining (A.34) with (A.25) yields, on recalling (2.11), that

$$\begin{aligned}
\sum_{\ell \in \{1, \dots, 4, 8, 12, 14\}} T_\ell = & - \left\langle \Delta_s [\alpha(\mathbf{c}) (\boldsymbol{\varkappa} - \overline{\boldsymbol{\varkappa}}(\mathbf{c}))] + \alpha(\mathbf{c}) (\boldsymbol{\varkappa} - \overline{\boldsymbol{\varkappa}}(\mathbf{c})) |\nabla_s \vec{\nu}|^2 - b(\boldsymbol{\varkappa}, \mathbf{c}) \boldsymbol{\varkappa}, \vec{\chi} \cdot \vec{\nu} \right\rangle_{\Gamma(t)} \\
& - \left\langle \nabla_s \cdot ([\boldsymbol{\varkappa} \underline{\text{Id}} + \nabla_s \vec{\nu}] \nabla_s \alpha^G(\mathbf{c})), \vec{\chi} \cdot \vec{\nu} \right\rangle_{\Gamma(t)} \\
& + \left\langle [b, \mathbf{c}](\boldsymbol{\varkappa}, \mathbf{c}) + (\alpha^G)'(\mathbf{c}) \mathcal{K} \nabla_s \mathbf{c}, \vec{\chi} \right\rangle_{\Gamma(t)}. \tag{A.35}
\end{aligned}$$

Summing (A.35) and (A.26) yields the strong form (2.4).

Finally, (3.27b), (2.5), (A.20), (2.10) and (2.13) immediately yield (1.10b).

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